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Framework for Development of General Models

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This report presents a framework for the development of a model for predicting the indoor air pollutant concentrations in a variety of building types under practical conditions of weather, building occupancy, building construction and pollutant source strength. The general concepts needed for developing an indoor air quality model are treated. Examples of the current state of indoor air quality models are given. The pollutants discussed are formaldehyde, radon, nitrogen oxides, tobacco smoke, particulates, carbon dioxide, and carbon monoxide.

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INDOOR AIR QUALITY MODELING PHASE I REPORT FRAMEWORK FOR DEVELOPMENT OF GENERAL MODELS

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ABSTRACT

This report presents a framework for the development of a model for predicting the indoor air pollutant concentrations in a variety of building types under practical conditions of weather, building occupancy, building construction and pollutant source strengths. The general concepts needed for developing an indoor air quality model are treated. Examples of the current state of indoor air quality models are given. The pollutants discussed are formaldehyde, radon, nitrogen oxides, tobacco smoke, particulates, carbon dioxide, and carbon monoxide.

Key Words: Indoor air pollution; modeling; air pollutants; environmental parameters; model concepts.

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Indoor Air Quality Modeling
Phase I Report
Framework for Development of General Models

1. Introduction

Purpose: The purpose of this report is to present a framework for a model which will allow the prediction of air pollutant concentrations in a variety of building types under practical conditions of weather, building occupancy, building construction, and pollutant source strengths. The model will provide concentrations of several important pollutants and include both temporal and spatial variations of contaminants.

Need: Since there are nearly 90 million dwelling units and approximately four million other occupied buildings in the U.S., it appears impractical to obtain enough field data to adequately assess the status of the important pollutants and their distribution in this large number of buildings. Almost all of them will have differences in their environments, construction details and occupancies which will affect pollutant concentrations. This will make predictions based upon a limited number of studies and observations very difficult. A reliable prediction model is needed to assess the extent and seriousness of the indoor air quality problem for a variety of buildings under different occupancy and environmental conditions.

A validated prediction model is needed so that a national program for improved indoor air quality may be economically developed which makes use of results of field tests and health effects research. Health effects research and field studies will be done outside the scope of this project.

There are several other uses for a model in the complex area of indoor air quality research. In the short-term, a model will assist in:

1. The design of field and laboratory tests. What to measure, where and how often, for example, so tests by several investigators can be better coordinated.

2. Evaluation of instrument requirements. What accuracy, what time constant, integrating or continuous, etc.

3. Evaluation of existing experimental data for use in data bases.

4. Evaluation of data collected for suitability in data bases.

5. Providing methods whereby various investigators using different models may produce consistent results.

In the longer term, a model will be useful for:

1. Evaluation of the effectiveness of various indoor air quality options, such as increased ventilation, heat exchangers, particulate and gaseous removal equipment, material substitution, and contaminant emanation

suppression techniques, as well as the evaluation of behavior modification and providing sensitivity analyses on various control methods for practical decision making.

2. Assisting in risk assessment studies for various pollutants by predicting exposures as they vary with time (peak and average) and space.

3. Providing practical information for the establishment of standards.

2. Concepts

Figure 1 shows a schematic diagram of the general problem to be solved. There must be, for any pollutant of interest, a source or sources. A source could be a concentration in the outdoor air, but more usually it would be from the surrounding earth or water supply, as in the case of radon, or from building materials and furniture, as in the case of formaldehyde or from personal habits of occupants such as smoking. A source may also be from equipment, combustion appliances and activities in the space, as in cooking, cleaning, etc. Source emanation into the indoor air is often complicated, being affected by indoor/outdoor weather conditions, HVAC equipment, peoples activities, etc. Much work has been done in source identification and the time variation of emanation [1-3].

Emanation from the source is introduced into the indoor air and is transported by convection and diffusion throughout the space, until it is removed from the air by outward air leakage, deposition on surfaces in the space, removal by HVAC equipment or modified by chemical or other action. There is some knowledge of these mechanisms for many pollutants [1].

Pollutants are then exposed to people in various activities as they move into, through and out of that space, resulting in a personal exposure for each person depending on his movement and activity.

This exposure then results in a personal dose of the pollutant. The dose, in general, will be less than the concentration-time integration since the person will have some natural defense mechanisms which reduce the dose [4].

The personal dose then produces an effect on the person, which may be only an annoying odor, with no further effect. Odors are of interest to the HVAC engineer, since human comfort is involved. It is supposed that odors can affect human performance in some situations, and therefore they should be a public health concern [5]. The pollutant may cause an acute health effect, such as eye irritation or coughing, with no long-term effect after the pollutant is removed. Many pollutants are suspected or proved to have chronic effects, such as lung cancer in the case of radon. Such chronic effects may take decades to appear in people [6].

The model contemplated in this study will be concerned with only the first three blocks of Figure 1. It will be confined to the identification of the sources, their transport and removal, and the resulting time and spatial contaminant concentration predictions. It is expected that, if successful, the concentration predictions can be extended to obtain personal exposures by adding various scenarios of a persons time, position and, activities in the space of interest.

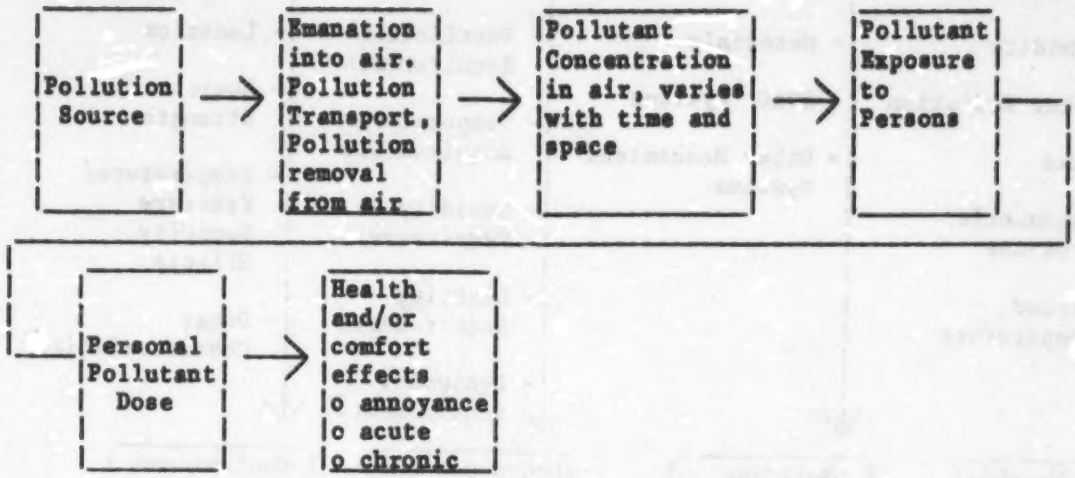

Pollution Source
Emanation into air. Pollution Transport, Pollution removal from air
Pollutant Concentration in air, varies with time and space
Pollutant Exposure to Persons
Personal Pollutant Dose
Health and/or comfort effects
o annoyance
o acute
o chronic

Diagram of the General Indoor Pollution Problem

Figure 1

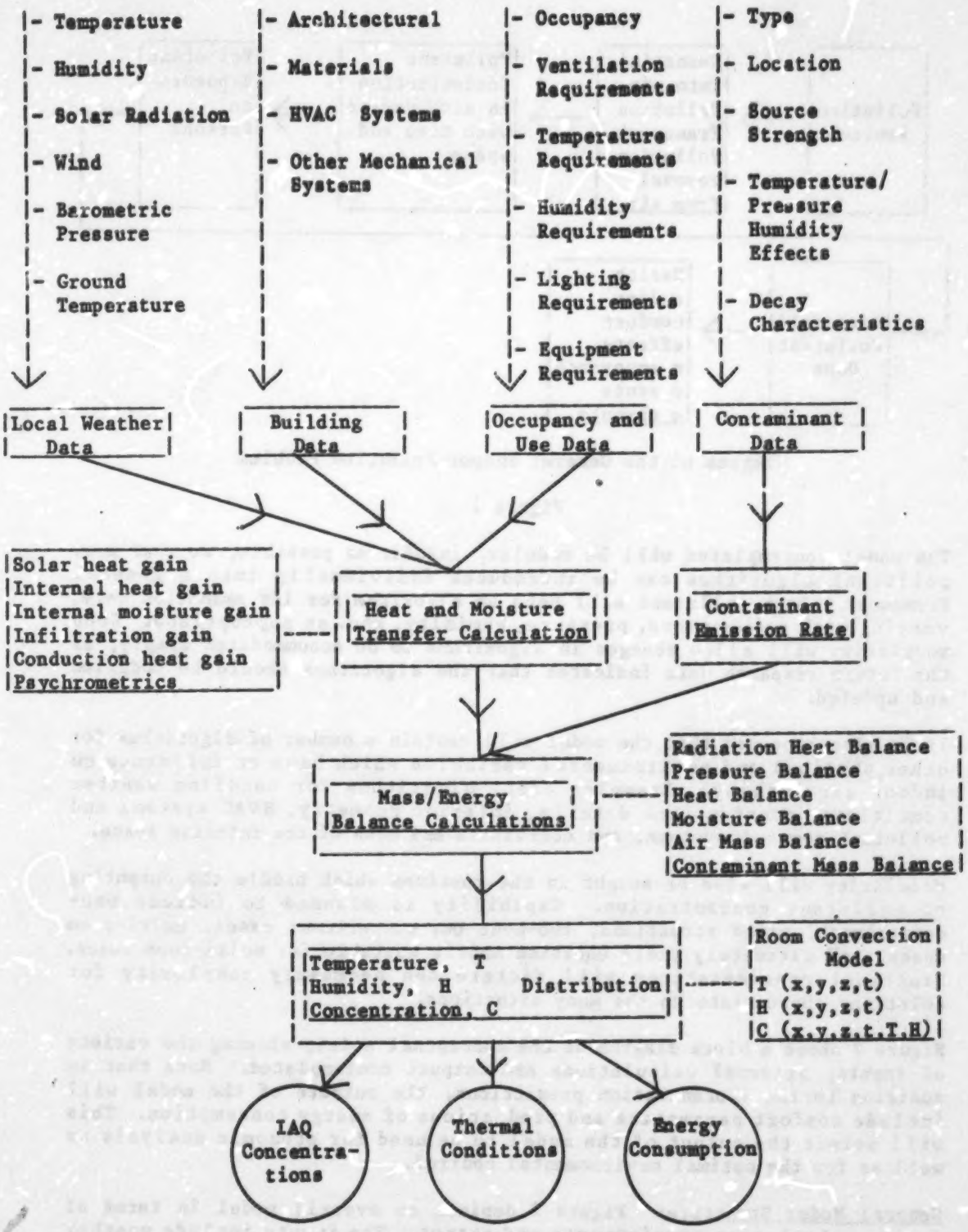
The model contemplated will be modular, insofar as possible, so that many pollutant algorithms can be introduced individually into a general framework. Each pollutant will have an algorithm for its emanation rate, varying with temperature, pressure, humidity, etc. as appropriate. Such modularity will allow changes in algorithms to be accommodated simply, if the future research data indicates that the algorithms should be modified and updated.

It is also expected that the model will contain a number of algorithms for other physical and environmental variables which have an influence on indoor air quality. Examples are: Algorithms for handling weather conditions, construction details, interior geometry, HVAC systems and pollutant removal systems, and activities and uses of the interior space.

Modularity will also be sought in the routines which handle the outputing of pollutant concentration. Capability is planned to include one-compartment, mixed situations, two-node one-compartment cases, multi-room cases, and ultimately field equation models suitable for multi-room cases. Practical considerations will dictate the necessary complexity for solutions appropriate to the many situations.

Figure 2 shows a block diagram of the conceptual model, showing the variety of inputs, internal calculations and outputs contemplated. Note that in addition to the concentration predictions, the outputs of the model will include comfort parameters and predictions of energy consumption. This will permit the output of the model to be used for economic analysis as well as for the optimal environmental control.

General Model Structure: Figure 2 depicts an overall model in terms of input, calculation requirements and output. The inputs include weather parameters, building architectural data and occupancy data as well as the contaminant source information. This extensive set of input data is



Block Diagram of the Model Concept

Figure 2

required to accurately assess the strong interactions between the building thermal environment and emanation and migration of the pollutants. Because of the fact that emission and decay rates of many contaminants are considered dependent upon their ambient temperature, humidity and air motion, the prediction of the contaminant concentration level at a given point in the building at a given time necessitates the simultaneous determination of these environmental properties for the air as well as the surface temperature and surface moisture content of the interior furnishings. This applies not only to the detailed calculations for air, moisture and heat transfer through the building envelope, but also to the accurate energy and mass balance analysis between the heat and moisture gain, considering the heating, cooling, humidifying and dehumidifying capacities of the HVAC systems and its control equipment. The heat and moisture storage capacity of the solid surfaces exposed to the room air must also be taken into consideration. Detailed and accurate calculation procedures are already available in the Thermal Analysis Research Program (TARP) of the National Bureau of Standards [1], which has been developed previously to simulate the hourly heating and cooling requirements of the building.

On the other hand, mass balance models for various contaminants have been developed by several authors to predict the contaminant concentrations in spaces as functions of source strengths, decay rates and dilution rates. These will be discussed in more detail in section 4. All of these existing models however, are applicable where the room air is well mixed so that its temperature, humidity, contaminant concentration and air velocity are all uniform throughout the space. While this single node assumption may be adequate for assessing the effect of time average values for a day or for a longer period, these models fail to account for the localized peak concentrations of certain contaminants, which are sometimes considered more critical for health effects than the long time and overall average exposures [7].

For the risk assessment of individuals, information is needed for the time-frequency data of the contaminant concentration for a period of time at a prescribed location in the building. Based upon these data, appropriate control strategies, such as the installation of air filters, increased ventilation, alteration of HVAC systems and/or interior furnishing, etc. will have to be developed to modify the time-frequency profile. These control strategies are, however, all costly and they must take into account economic trade offs with respect to risk. The economic analysis, in turn requires the accurate data for building materials, internal furnishings, HVAC and air cleaning equipment and air handling systems and the energy costs, maintenance, etc.

Although the model structure shown in figure 2 is designed to address all of these complex and interwoven aspects of building thermal performance and indoor air quality, it must be emphasized that it does not necessarily depict actual flow of the calculation algorithms. In fact the three sequential blocks, heat and moisture transfer calculation, mass/energy balance calculation and temperature/humidity/concentration determination should ideally be handled in a single block, provided that the efficient parallel processing algorithms are developed for modern high speed computers.

Expected Model Capabilities: Although comprehensive in scope, the model is expected to be simple to use due to its modular structure. In this way, predictions of concentrations can be made for a number of cases by selecting the appropriate algorithms for a specific pollutant for specific buildings under specific operating conditions, etc. from an extensive menu, inserting them in the framework, and exercising the model. If this can be accomplished, the model will be valuable in providing information to fulfill the purposes outlined above.

Limitations: In order to provide a manageable scope to this very extensive problem, certain limitations are necessary. The model results will be pollutant concentration predictions in interior spaces, with appropriate time and spatial variations. Personal exposures will not be included, but will be left to others. Climate and building types and interior uses will be limited to some extent. These limitations will be determined during subsequent work. It is expected that enough variety to cover all important situations will be included. Only certain pollutants will be included. A list, and discussion and rationale for pollutant selection or rejection will be given below.

3. Parameters Included

Pollutants, sources and sinks: The following pollutants to be considered were agreed to in the workshop held at NBS in February 1985 [8]. The order of the pollutant in the listing is not necessarily in order of importance.

Radon - The first radioactive decay product of radium, radon is a gas which can diffuse into buildings. Further decay products are adsorbed on particles which can lodge in the lung, where subsequent alpha particle emissions can cause lung cancer. The most important source is the earth around buildings, although well water in some locations is an important source [9,10].

The source strength depends upon soil radium concentration, soil permeability, pressure differences and perhaps temperature. No validated algorithms exist. Both point and area sources may be involved.

The radon decays and forms solids which are attracted to and attach to other dust particles, and are ultimately removed with the dust. The process is well established, and though complex, some algorithms have been developed, and others can be developed [11].

The spatial distribution algorithms are needed, but the process is controlled by diffusion, convection and gravity. Therefore algorithms may be developed employing other particle removal mechanisms.

Formaldehyde is widely used in many building products, furniture and clothing. It is clearly an irritant, causing annoyance and acute eye and respiratory affects. It is suspected of being a human carcinogen [12].

The source strength [13] depends upon area, temperature, humidity, source material, and time. Although complex, considerable laboratory and field work has been done, and algorithms are well advanced [13].

The natural removal mechanisms of reactions with other substances in the air, absorption in and desorption from materials occur, but models are not yet developed. Water and water vapor as a potential sink, needs to be considered.

Nitrogen Oxides, (NO_2 and NO) - NO_2 and NO are suspected of causing acute health effects [7]. The sources are combustion processes causing nitrogen-oxygen reactions in air at high temperatures.

Source strengths, from point sources, such as gas ranges and other unvented combustion appliances are well developed [14]. Manufacturers are developing appliances with lower NO_2 production, which will affect source strengths in the future [7].

There is some evidence of decay or chemical reaction of NO_2 and NO with materials in spaces, but no models exist.

Tobacco Smoke - The health effects of tobacco smoke on smokers is well known [15]. The effects of sidestream smoke on non-smokers has received much attention, and recent research [16] suggests effects on the respiratory tracts of children exposed. Increased probability of lung cancer in spouses of smokers has also been indicated [16].

Tobacco smoke is a very complex mixture of particles and gases. Good particulate models exist, but gaseous models need development to provide optimal source strength algorithms.

Tobacco smoke does decay with time, due to natural particulate removal, agglomeration and gaseous absorption, but better models are needed.

Particulates (other than tobacco smoke, including biomatter and allergens) - other particulates, from household activities, office machines, etc. should also be considered. Little is known about the source strengths. Some allergens enter spaces with outdoor air. Some models can be developed which may be useful in estimating source strengths.

Natural removal mechanisms, settling, agglomeration, deposition, chemical reactions, and resuspension need considerable model development, although some models exist. As seen below, this project will not include micro-organisms and allergens per se.

Carbon Dioxide (CO_2) - CO_2 is not suspected to be a comfort or health hazard, per se, but is included here because it has been suggested as an indicator of other pollutants more difficult to measure [17]. Principal sources are human metabolism, which is well modeled, and combustion processes, which are also well modeled. Absorption and desorption may occur, and are not well modeled.

Carbon Monoxide (CO) - The health effects of CO are well known, and good models exist [18] provided the source strengths are known. The model should be capable of handling CO.

Water Vapor (H_2O) - H_2O is not a pollutant, per se, but good models do exist. The effects of water vapor levels on other pollutants is needed for completeness. These effects need considerable study.

The following pollutants were considered by the workshop [8] and were set aside from this study for various reasons. Some were felt impractical to model with current knowledge, others (asbestos) were being handled separately, or research was not advanced far enough for consideration in the model.

Volatile Organic Compounds (VOC) (other than tobacco smoke and formaldehyde) - A wide variety emanate from a muliplicity of sources. Health effects of only a few have been studied.

Sulfur Dioxide (SO_2) - The sources are mainly from combustion of wood, coal and impure kerosene. The sources are highly variable and not predictable enough to be modelled.

Pesticides - Source strength and removal mechanisms are not well known.

Micro-Organisms and Allergens - Although these are very important, the necessary knowledge of source strength, removal and health effects need much further study.

Ozone (O_3) - O_3 was not felt to be an important indoor pollutant for buildings by the workshop participants [8].

Asbestos - Asbestos was not included, since it is being handled separately as a specific public health problem.

In addition to the specific pollutants to be included in the model, the following parameters should be included in the model where appropriate.

Generic sources of pollution -

- People, machines and peoples' activities
- Building materials and furnishings
- Consumer products
- HVAC equipment
- Outdoor air
- Water supply
- Combustion products

Source Strength Variations - The model should be able to handle the following important parameters affecting some emanation rates -

- Environmental factors - Time variations should be handled in appropriate time steps so that necessary detail on peak and average pollutant concentrations can be obtained. Effects of temperature, humidity, pressure, air movement, etc. should also be considered.

- Point sources, such as unvented kerosene heaters should be considered.

- Area sources, such as emanation from wall coverings, carpets, etc. should be handled.

- The effects of permeation barriers, such as paints on plywood or particle board should be considered.

- Volume sources, such as the production of radon daughters from radon in the air should be considered.

Other parameters: Parameters other than the pollutants which must be considered in order to provide predictions of indoor pollutant concentrations are listed below.

Weather - Local temperature, humidity, wind, solar radiation, pressure, and ground temperature should be included. Correlation of nearest weather station data with local conditions may sometimes be possible.

Architectural details - Building design, spatial relation of interior spaces, doors and other openings between spaces, envelope details, and building materials should be covered. Furnishings and other interior treatments, and machines and processes in buildings must be known and considered.

HVAC systems - The means of control of temperature, humidity, etc. involving heating, cooling, humidification and dehumidification should be known, as well as the equipment for removal of contaminants, both particulate and gaseous. The model is expected to simulate typical HVAC systems and equipment commonly found in residential as well as commercial buildings.

Ventilation - The operation of the HVAC system in providing ventilation must be known, as well as infiltration, natural ventilation and any local intakes or exhausts. The outlets and returns in all spaces must be known so local mixing and ventilation effectiveness can be predicted.

Within space conditions - The model should handle environmental parameters (temperature, humidity, air motion) as well as concentration predictions for:

1. Mixed air in a single zone
2. Mixed air in a 2 node single zone
3. Field equations in a single zone
4. Multizone (vertical and horizontal) adjacent spaces

Various time steps should also be possible with small enough time step capability to predict peak concentrations for some pollutants.

The building occupancy and operating schedules are also necessary, covering lighting, HVAC systems, other equipment, temperature, set points, etc.

4. Review of Existing Models

In this section, brief reviews of several models will be given. It is not possible to cover all models here, but those mentioned are those chosen as being most appropriate for use in the general IAQ model.

4.1 Formaldehyde Emission Rate Models

On the basis of surface emission rates of underlayment, paneling and medium-density fiberboard at different combinations of temperature, relative humidity (RH), and ambient formaldehyde (HCHO) concentrations, Oak

Ridge National Laboratory (ORNL) [13] developed models that can predict surface emission rates at nearby values of these parameters once the surface emission rate at 23°C, 50% RH, and 100 ppb HCHO concentration is determined. At any given temperature and RH, surface emission rate and HCHO concentration obey the following equation relating the ambient and a bulk layer of air, each containing different HCHO concentrations:

$$S = a + b \cdot C \qquad (1)$$

where S = HCHO surface emission rate, $mg/m^2 \cdot h$
a = linear regression intercept giving HCHO surface emission rate at C = 0 ppb, $mg/m^2 \cdot h$
b = linear regression slope, $mg/m^2 \cdot h/ppb$
C = HCHO concentration, ppb

The model developed by ORNL [13] predicts the ratio of S to S_{std}, (its value at standard conditions, 23°C, 50% RH and 100 ppb HCHO concentration).

$$\frac{S(T,RH,C_V)}{S_{std}} =$$

$$\frac{[1+B(T-296)] \cdot [1+E(RH-50)] \cdot [e^{-C(\frac{1}{T} - \frac{1}{296})} \cdot (RH/50)^A \cdot C_{B_{std}} - C_V]}{C_{B_{std}} - 0.1} \qquad (2)$$

where S = HCHO emission rate (mg/m^2h)
std = standard test conditions (i.e., 23°C, 50% RH, C_V = 0.1 ppm)
T = temperature (K)
RH = relative humidity (%)
A,B,C,E = model coefficients for temperature and RH terms
C_B = HCHO concentration in the bulk phase (ppm)
C_V = HCHO vapor concentration (ppm)

for T = 23°C and RH = 50%, equation 2 reduces to:

$$\frac{S(C_V)}{S_{std}} = \frac{C_{B_{std}} - C_V}{C_{B_{std}} - 0.1}$$

Equation 2 contains five coefficients: A, B, C, E, and $C_{B_{std}}$. The best fit of these to measured data were determined by ORNL. Table 1 gives values of the five coefficients for paneling, underlayment, and medium-density fiberboard. (No physical meaning should be attributed to any of the coefficients even though one of them, $C_{B,std}$, is supposed to correspond to the bulk phase HCHO concentration. The values of the coefficients are determined by numerical regression, not by any physical measurements, and the model itself is an empirical one.)

The National Bureau of Standards (NBS) tested this model in a controlled-environment chamber. The surface emission rates of paneling, underlayment, and table tops made of medium-density fiberboard were measured at 23°C and 50% RH at various air exchange rates -- and hence various HCHO concentrations -- in specially constructed medium-sized measuring chambers.

The coefficients of equation 1 were determined by linear regression analysis and S_{std} was calculated for each specimen. The specimens, except for several used as controls, were then placed into a prototype house located in the controlled environment chamber to see how well HCHO concentrations under more "real" conditions could be predicted from measurements of individual specimens. Two underlayment specimens had to be cut in order to cover the floor of the house. (The results of the house study are not discussed here.) The specimens were then removed from the prototype house and remeasured in the medium-size chambers to see if the functions relating surface emission rates to HCHO concentrations were stable. The experiments in the controlled environment were repeated at 26° and 60% RH. Resulting values of S/S_{std} under both sets of conditions were compared with predictions of the ORNL models [13]. As an illustration, we will present the results currently available for underlayment. For underlayment, the ORNL models, using equation 2 and the coefficients in table 1, are:

$$S/S_{std} = 1.38 - 0.0038 \cdot C \text{ at } 23^{\circ}C, 50\% \text{ RH}$$
$$S/S_{std} = 2.54 - 0.0048 \cdot C \text{ at } 26^{\circ}C, 60\% \text{ RH} \qquad (3)$$

The NBS results for uncut underlayment are best fit by the following equations:

$$S/S_{std} = 1.69 - 0.0069 \cdot C \text{ at } 23^{\circ}C, 50\% \text{ RH before placing in the house}$$
$$S/S_{std} = 1.61 - 0.0061 \cdot C \text{ at } 23^{\circ}C, 50\% \text{ RH after placing in the house} \qquad (4)$$
$$S/S_{std} = 3.21 - 0.0087 \cdot C \text{ at } 26^{\circ}C, 60\% \text{ RH before placing in the house}$$

The NBS results for cut underlayment are best fit by the following equations:

$$S/S_{std} = 1.69 - 0.0068 \cdot C \text{ at } 23^{\circ}C, 50\% \text{ RH before placing in the house}$$
$$S/S_{std} = 1.60 - 0.0060 \cdot C \text{ at } 23^{\circ}C, 50\% \text{ RH after placing in the house} \qquad (5)$$
$$S/S_{std} = 3.12 - 0.0069 \cdot C \text{ at } 26^{\circ}C, 60\% \text{ RH before placing in the house}$$

Table 1
Nonlinear Regression Analysis for
ORNL HCHO Surface Emission Rate Model

Pressed-wood Product	C	A	B_{std}^{C}	B	E
Particleboard Underlayment	9400	0.37	0.36	0.025	0.016
Paneling	6500	0.66	0.41	0.053	0.029
Medium Density Fiberboard	5000	1.90	0.90	0.090	0.000

The NBS results and the predictions of the ORNL model are shown in figure 3. The magnitude of the slopes predicted by ORNL is about 40% smaller than those found by NBS.

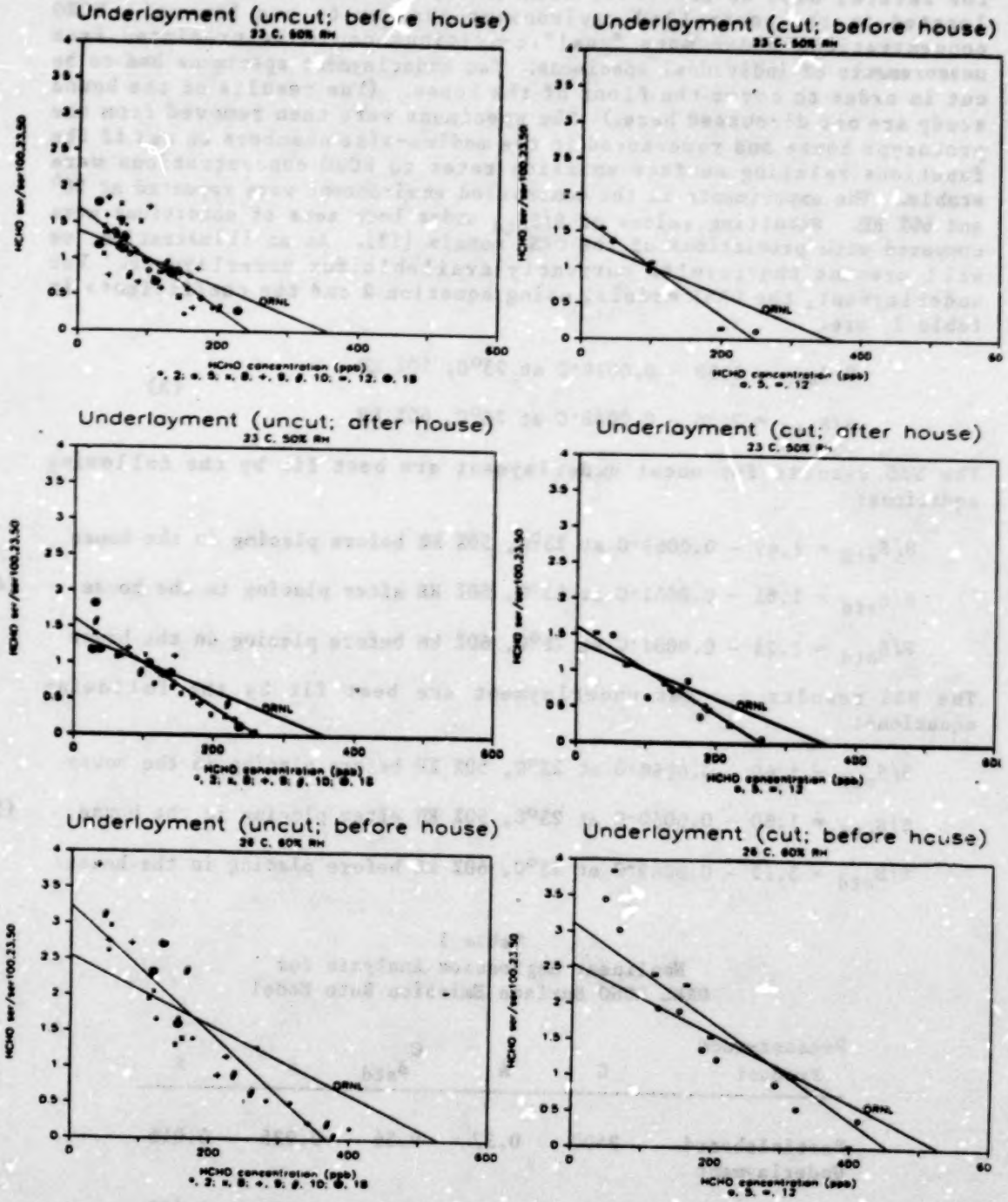


Figure 3. Measured underlayment surface emission rates of formaldehyde compared to ORNL's model (predicted by equation 2 using coefficients in table 1).

4.2 Radon Emission and Decay Models

General radon emission rate models are not yet available. The Lawrence Berkeley Laboratory (LBL) [10] has done considerable work on this and useful models may be developed soon. However, radon and radon progeny models have been developed, to predict decay rate as it occurs in the indoor air [11].

4.2.1 NBS's model

A physical model for the dependence of radon decay on ventilation can be expressed by the equations [11]:

$$\frac{dA_0}{dt} = Q - (\lambda_0 + I)A_0 + IA_0^o \qquad (6)$$

$$\frac{dA_i}{dt} = \lambda_i A_{i-1} - (\lambda_i + I)A_i + IA_i^o \text{ for } 1 \leq i \leq 4 \qquad (7)$$

where A = activity concentration of the radionuclide (pCi/L)

Q = entry rate of radon (pCi/L·h)

λ = radioactive decay rate (h^{-1})

I = infiltration rate (h^{-1})

t = time (h)

Subscript "i" refers to the i^{th} radionuclide (i = 0 to 4)

Superscript "o" refers to outdoor air.

Kusuda et al. [11] solved this set of equations for several typical combinations of I and Q and presented the results in terms of equilibrium total alpha particle energy concentration of radionuclides, $\bar{E}$;

$$\bar{E} = \sum_{i=1}^{N} C_i A_o \qquad (8)$$

where C_i's are predetermined constants representing potential alpha energy per pC_i of each radionuclide. Using the unit of working level, WL, details of which are found elsewhere (see for example reference 11), equation (8) can also be expressed as

$$\bar{E} = \frac{A_o}{100 pC_i L^{-1}} WL \qquad (9)$$

4.2.2 Geomet's model

In research on indoor air quality Nagda et al. [18], developed the

following model for predicting the indoor level of radon in equation 10,

$$\frac{dC_{in}}{dt} = \frac{ES_e}{V} + \frac{q}{V} + I\,(\alpha_o C_{out} + \alpha_s C_s) - IC_{in} - \lambda^o C_{in} \qquad (10)$$

where C_{in} = indoor concentration (atoms/m^3)

E = radon flux density per unit surface (atoms/h m^2)

S_e = exhaling surface area (m^2)

V = volume (m^3)

q = radon release rate from indoor source (i.e., water, etc.)

C_{out} = outdoor concentration (atoms/m^3)

I = air exchange rate (h^{-1})

α_o = fraction of external air coming from outdoors

α_s = fraction of external air coming from soil; $\alpha_o + \alpha_s = 1$

λ^o = radon decay rate (h^{-1})

4.2.3 Radon Progeny Models

The activity concentration indoors of the new generation of free radon progeny, A_f^i, and attached radon progeny, A_a^i, may be stated as follows [9]:

$$\frac{dA_{f,in}^i}{dt} = I A_{f,out}^{i-1} + \lambda^i A_{f,in}^{i-1} + R^{i-1}\,\lambda^i A_{a,in}^{i-1} - (I + \lambda^i + \chi + \lambda^p) A_{f,in}^i$$

$$\frac{dA_{a,in}^i}{dt} = A_{a,out}^i + \lambda^i (1-R^{i-1}) A_{a,in}^{i-1} + \chi A_{f,in}^i - (I + \lambda^i + \lambda^d) A_{a,in}^i \qquad (11)$$

where I = air exchange rate (h^{-1})

λ^i = radioactive decay constant for ith progeny (pCi/L·hr)

R = recoil factor to define detachment

χ = attachment rate

λ^p = deposition constant for free progeny (plateout)

λ^d = deposition constant for attached progeny

and subscript "in" and "out" refer to inside and outside air.

The mass balance for a given generation of radon progeny is determined by:

$$\frac{dA^i_{in}}{dt} = \lambda^i A^{i-1}_{in} - (\lambda^i + I + \lambda_s) A^i_{in} + IA^i_{out} \qquad (12)$$

where λ_s is the settling rate.

4.3 NO_2 Emission Rate Models

NO_2 emission rate models have been developed. However, the NO_2 emission from combustion under various conditions needs refining. For example, a range burner flame, heating a pan of food from a cold start, produces NO_2 at a rate which varies with time. Many measurements have been made [7] [18] (see Figures 4 and 5), but general predictive models for NO_2 generation are not yet available. In addition, NO_2 does react with unknown materials in the environment at rates which are equivalent to air exhange rates from zero to 0.5. NO_2 models of Geomet and Harvard [18] [19] are given for kerosene heaters and gas ranges.

$$\frac{dC}{dt} = I(C_{out} - C) - kC + S \qquad (13)$$

where C = the concentration of NO_2 indoors ($\mu g\ m^{-3}$),

I = air exchange rate (h^{-1})

C_{out} = concentration of NO_2 outdoors ($\mu g\ m^{-3}$),

S = indoor emission rate of NO_2 ($\mu g\ m^{-3}\ h^{-1}$),

k = first-order decay constant (h^{-1})

t = time (h)

$$C(t) = (1 - e^{-I't}) \frac{S'}{I'} + C^o e^{-I't} \qquad (14)$$

where C(t) = the concentration of NO_2 indoors ($\mu g/m^3$),

$I' = I + k$,

$S' = S + IC_{out}$, and

C^o = the concentration of NO_2 indoors at time t_o

The exposure in a time interval (t_1, t_2) is given by

$$E(t_1,t_2) = \int_{t_1}^{t_2} C(t)dt = C\,(t_2 - t_1) + \frac{C^o - C}{I'} (e^{-I't_1} - e^{-I't_2}). \qquad (15)$$

where $E(t_1,t_2)$ is the exposure between time t_1 and time t_2, and
$C = S'/I'$, the steady-state indoor NO_2 concentration.

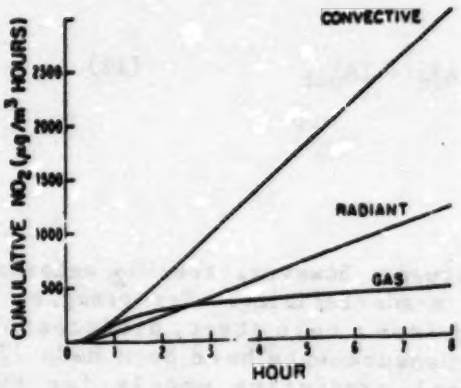


Figure 4. Predicted NO_2 concentrations from a convective kerosene heater, a gas stove and a radiant kerosene heater with I = 0.0 ACH

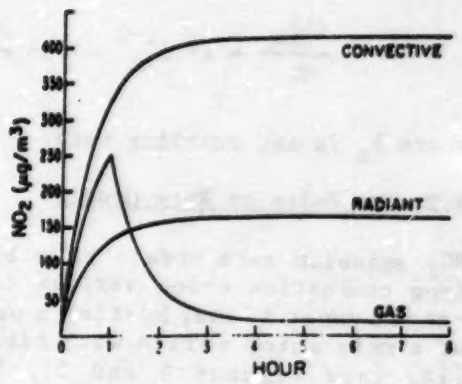


Figure 5. Predicted NO_2 concentrations from a convective kerosene heater, a gas stove and a radiant kerosene heater with I = 1.0 ACH

4.4 Tobacco Smoke Models

Tobacco smoke particle emission rates have been intensively measured. Emission rates vary with the types of cigarettes, and how individuals smoke them.

However, for purposes here, Repace [16] indicates that particulate generation per cigarette may be taken as 24 mg per cigarette ± 20%. Repace also has examined tobacco smoke agglomeration and aging. The data showed that when smoking continues, the new smoke tends to predominate, so good approximations may be made by neglecting aging.

4.5 CO_2 Emission Rate Models

Generally CO_2 emission models are well developed, depending particularly on the amount of carbon burned, or average metabolic measurements on people. CO_2 is non-reactive after introduction into the environment.

4.6 CO Emission Rate Models

CO is also non-reactive in the environment. However, its emission models are known only for specific cases (cigarettes, specific combustion burner situations, etc). Harvard [14] and LBL [7] have done considerable work, but no general model exists to predict CO generation [19] from a wide range of sources.

4.7 Water Vapor Models

Water vapor (H_2O) is important to consider here, since it reacts with many pollutants in the air. Emission rate models are well developed for many cases (metabolism and perspiration of people, evaporation from cooking, showering and bath taking, humidifiers, etc.). However, H_2O is adsorbed and desorbed in and from building materials and furnishings. Tsuchiya [20] and later Kusuda and Miki [21] used a mass balance equation similar to equation 10 to predict indoor air moisture content and obtained good agreement with measured results. The absorption and desorption of H_2O by

interior surfaces of buildings and internal furnishings is extremely important as it is also believed to affect the emission characteristics of other pollutants.

4.8 Building Air Movement Models

The simplest and most widely used model to predict space concentration assumes uniform mixing in the space or spaces under consideration. This is referred to as a one-node model in this report. See Figure 6.

Assuming complete mixing of the incoming air with the room air, the mass balance of a pollutant in a single room may be written as eq. (16).

$$V\frac{dC_i}{dt} = (q_o + q_2)C_o - (q_1 + q_2)C_i + S - R \qquad (16)$$

Since the mixing of the incoming air with the room air is not uniform, a mixing factor (k) is used to account for the effect. This can be accounted for by considering the equations below.

Air mass balance: $q_o + q_2 = q_3 + q_4$

Pollutant mass balance: $V\frac{dCi}{dt} = kq_oC_o(1-F_o) + kq_1C_i(1-F_1) \qquad (17)$

$$+ kq_2C_o - k(q_o + q_1 + q_2)C_i + S - R$$

In equations (16) and (17)

C_i = concentration indoors,

C_o = concentration outdoors,

t = time,

q_o = volumetric flow for make-up air,

q_1 = volumetric flow for recirculation,

q_2 = volumetric flow for infiltration,

q_3 = volumetric flow for exfiltration,

q_4 = volumetric flow for exhaust,

F_o = filter efficiency for make-up,

F_1 = filter efficiency for recirculation,

V = room volume,

S = indoor source emission rate,

R = indoor sink removal rate

k = mixing factor

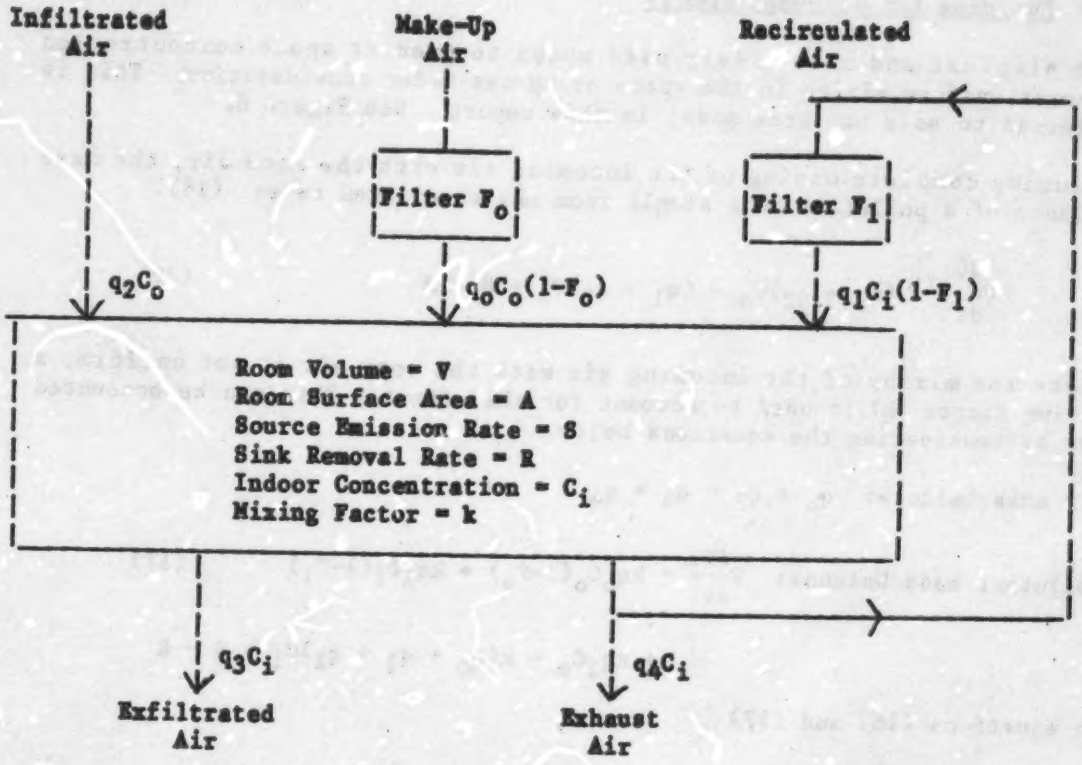


Figure 6. Schematic representation of a Single-Compartment Indoor Air Quality Model

The solution of the equation for the change in C_i with t, holding all other factors constant and with boundary values $C_i = C_s$ at $t = 0$, is

$$C_i = \frac{[k[q_o(1 - F_o) + q_2]C_o + S - R]}{k(q_o + q_1F + q_2)} [1-e^{-(k/V)(q_o+q_1F_1+q_2)t}] \quad (18)$$

$$+ C_s e^{-(k/V)(q_o + q_1F_1+q_2)t}$$

This one-node model is easily extended to more than one connected space, as shown in figure 7.

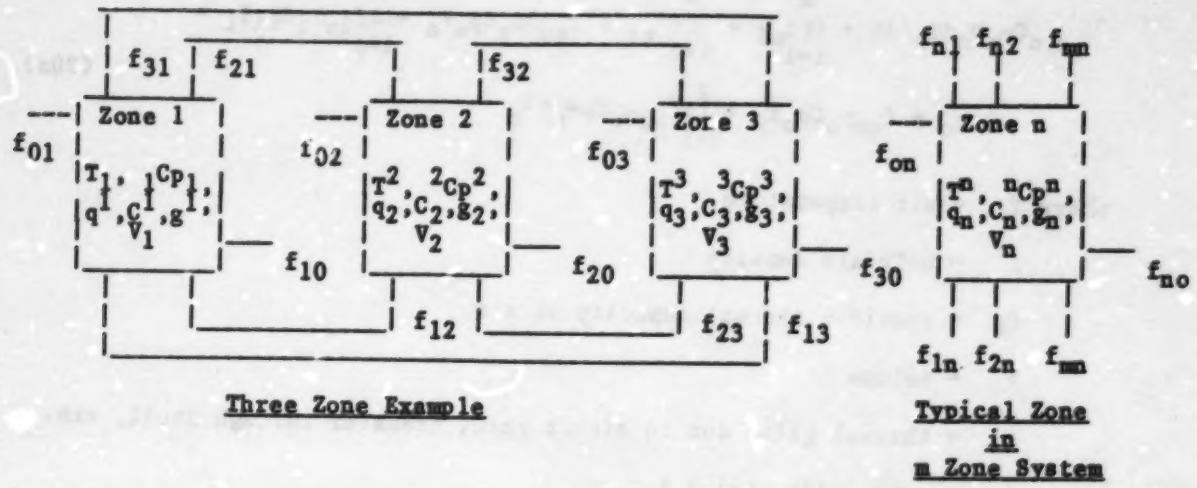
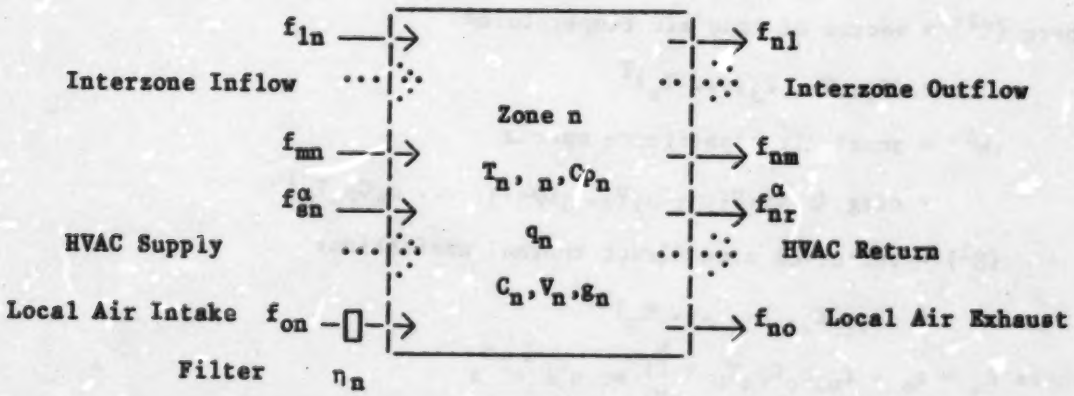


Figure 7. Three Zone One-Node Model

In general, airflow from any one zone to another must be considered. Define a flowrate variable, f_{ij}, the interzone volumetric airflow rate, such that f_{ij} indicates the volumetric flow rate from zone i to zone j (it is understood that $f_{ii} = 0.0$). Outdoor air exhaust and intake must be considered, f_{no} and f_{on}, and HVAC supply and return, f^{α}_{sn} and f^{α}_{nr}, local to each zone, where each zone may be served by several HVAC systems, $\alpha=1,2,\ldots,N$.



(For the equations derived below a thermal zone may be taken to have a very general meaning. An air duct and even an air system heating or cooling "plant" could, conceivably, be considered to be thermal zones.)

Thermal Equations

For a typical zone `n' within this building system equillibrium is necessary;

$$\rho_n Cp_n V_n dT_n/dt + (\sum_{i=1}^{m} f_{ni} + \sum_{\alpha=1}^{N} f^{\alpha}_{nr} + f_{no})\rho_n Cp_n T_n - \sum_{i=1}^{m} f_{in}\rho_i Cp_i T_i =$$

$$q_n + f_{on}\rho_o Cp_o T_o + \sum_{\alpha=1}^{N} f^{\alpha}_{sn}\rho_s Cp^{\alpha}{}_s T^{\alpha}{}_s \qquad (20a)$$

where T = air temperature

ρ = bulk air density

Cp = specific thermal capacity of air

V = volume

q = thermal gains due to direct gain, transfer through shell, etc.

i = zone index, i=1,2,3,...m

i=0 = outdoor index

r = HVAC return index

s = HVAC supply index

α = HVAC system index (for multiple HVAC systems)

or $$[M^2]\{dT^2/dt\} + \{Cp^2\}[F^2]\{T^2\} = \{E^2\} \qquad (20b)$$

where $\{T^2\}$ = vector of zone air temperatures

$= \{T_1, T_2, T_3, \ldots T_m\}^T$

$[M^2]$ = zonal air capacitance matrix

$= \text{diag}\ \{\rho_1 Cp_1 V_1, \rho_2 Cp_2 V_2, \rho_3 Cp_3 V_3, \ldots \rho_m Cp_m V_m\}$

$\{E^2\}$ = vector of zone direct thermal excitations

$= \{E_1, E_2, E_3, \ldots E_m\}^T$

where $E_n = q_n + f_{on}\rho_o Cp_o T_o + \sum_{\alpha=1}^{N} f^{\alpha}_{sn}\, {}_sCp^{\alpha}{}_s T^{\alpha}{}_s$

$[f^2]$ = mass airflow matrix

$$= \begin{bmatrix} F_{11} & -f_{21} & -f_{31} & \cdots & -f_{m1} \\ -f_{12} & F_{22} & -f_{32} & \cdots & -f_{m2} \\ -f_{13} & -f_{23} & F_{33} & \cdots & -f_{m3} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ -f_{1m} & \cdots & \cdots & \cdots & F_{mm} \end{bmatrix}$$

where $F_{nn} = (\sum_{i=0}^{m} f_{ni} + \sum_{\alpha=1}^{N} f^{\alpha}_{nr} + f_{no})$

$[f^2]$ is in general, asymmetric ($f_{ij} \neq f_{ji}$); zones need not exchange equal volumes of air

$\{Cp^2\}$ = vector of zone air specific thermal capacities

$= \{\rho_1 Cp_1, \rho_2 Cp_2, \rho_3 Cp_3, \ldots \rho_m Cp_m\}$

Continuity Equations: Positive Definiteness of $\{F\}$

Zonal Continuity

Within the assumption of incompressible flow, consideration of flow continuity requires that flow out of a zone must equal flow into the zone;

$$\sum_{i=1}^{m} f_{ni} + \sum_{\alpha=1}^{N} f^{\alpha}_{nr} + f_{no} = \sum_{i=1}^{m} f_{in} + \sum_{\alpha=1}^{N} f^{\alpha}_{sn} = f_{on} \qquad (21)$$

or $$\sum_{i=1}^{m} F_{nn} = f_{in} + \sum_{\alpha=1}^{N} f^{\alpha}_{sn} + f_{on} \qquad (22)$$

It then follows, since all airflow values are defined to be greater than or equal to zero, that the diagonal terms of the airflow matrix will always be greater than or equal to the sum of the off-diagonal terms in a row;

$$f_{nn} \geq \sum_{i \neq n}^{m} f_{ni} \qquad (23)$$

or if any infiltration or HVAC supply exists in the airflow system, then at least one of the diagonal terms will be strictly greater than the row sum, and the airflow matrix will be positive definite.

The zonal air capacitance matrix, $[M^2]$, is diagonal and positive, by definition. Thus the system of equations defined by equation (20b) may be solved when the airflow matrix, $[F^2]$, is positive definite, when infiltration or HVAC flow exists.

HVAC System Continuity

Flow continuity is required in the HVAC system(s);

$$\sum_{i=1}^{m} f^{\alpha}_{ir} - f^{\alpha}_{ro} = f^{\alpha}_{os} = \sum_{i=1}^{m} f^{\alpha}_{si} \qquad \text{for } \alpha=1,2,..,N \quad (24)$$

Flow-Pressure Equations (Momentum and Constitutive Relations)

While airflow between zones is physically driven by pressure differences it is useful to model airflow as either a prescribed function of time;

$$[F^2] = [F^2(t)] \qquad (25)$$

or as a pressure-driven flow;

$$[F^2] = [F^2(\{\Delta p\})] \qquad (26)$$

where $\{\Delta p\}$ = mean pressure differences between zones and from zones to the outdoor environment

$$\Delta p_{ij} = p_j - p_i \qquad \text{for } p_j > p_i$$

$$= 0.0 \qquad \text{for } p_j \leq p_i$$

In either case, the flow rates must satisfy the continuity requirement of equation (21).

Using prescribed flow rates, equation (25), an analysis may be conducted of indoor air quality for the common situation where forced convection driven by HVAC equipment dominates the flow without the need to consider pressure differences explicitly.

An accurate evaluation of pressure-driven flows, modeled by the second option, equation (26), that satisfy continuity, may be expected to be the most problematic aspect of the well-mixed zone model.

These flows may be due to bouyancy effects, wind induced pressures, and mechanically induced pressures and <u>may</u> be related to pressure differences using approximate, empirical expressions of the form;

$$f_{ij} = k_{ij}(\Delta p_{ij})^{x_{ij}} \qquad (27)$$

where the flow coefficients, k_{ij} and x_{ij}, depend upon the geometry of the flow boundary, and the nature of the flow, (laminar or turbulent, etc.).

Pressure differences due to bouyancy effects are critically dependent upon small differences in zone densities that are, strictly speaking, dependent upon temperatures and contaminant concentrations;

$$\rho_i = \rho_i(T_i, C_i) \qquad (28)$$

<u>Contaminant Dispersal Equations</u>

<u>Nonreactive Contaminants</u>

For a typical zone 'n' within this building system, contaminant mass equilibrium is necessary for each contaminant, k, of interest:

$$V_n dC^k{}_n/dt + \left(\sum_{i=1}^{m} f_{ni}\right) = \left(\sum_{\alpha=1}^{N} f^{\alpha}{}_{nr} + f_{no}\right)C^k{}_n - \sum_{i=1}^{m} f_{in} C^k{}_i =$$

$$g^k{}_n + f_{on}(1-\eta_n)C^k{}_o + \sum_{\alpha=1}^{N} f^{\alpha}{}_{sn} C^k{}_s \qquad (29)$$

where V = zone volume

C = contaminant concentration

g = contaminant generation rate

η = filter efficiency

k = contaminant type index

or $$[V^2]\{dC^{kz}/dt\} + [F^2]\{C^{kz}\} = \{S^{kz}\} \quad (30)$$

where $\{C^{kz}\}$ = vector of zone contaminant concentrations

$= \{C^k_1, C^k_2, C^k_3, \ldots C^k_m\}^T$

$[V^z]$ = zonal volume matrix

$= \text{diag}\{V_1, V_2, V_3, \ldots V_m\}$

$\{S^{kz}\}$ = vector of contaminant source rates

$= \{S_1^k, S_2^k, S_3^k, \ldots S_m^k\}^T$

where $S_n^k = g^k_n + f_{on}(1-\eta_n)C^k_o + \sum_{s=1}^{m} f_{sn}C^k_s$

Reactive Contaminants

If two contaminants, a and b, react to product a third species c;

$$a + b \rightarrow c$$

and the rate of production of c is dependent linearly upon the concentratons of a and b as;

$$dC^c/dt = R_{ab}(C^a, C^b) \quad (31)$$

where C = concentration and R_{ab} is the rate of production of c as a function of a and b

From the stoichiometry of the reaction;

$$(m_a)a + (m_b)b \rightarrow (m_c)c$$

$$m_a + m_b = m_c$$

where m = mass

it follows that;

$$dC^a/dt = -(m_a)/(m_a + m_b)\, dC^c/dt = -(m_a)/(m_a + m_b)R_{ab}(C^a, C^b)$$
and
$$dC^b/dt = -(m_b)/(m_a + m_b)\, dC^c/dt = -(m_b)/(m_a + m_b)R_{ab}(C^a, C^b) \quad (32)$$

or, defining;

$$g^{ab}(C^a, C^b) = -(m_a)/(m_a + m_b)R_{ab}(C^a, C^b)$$
$$g^{ba}(C^a, C^b) = -(m_b)/(m_a + m_b)R_{ab}(C^a, C^b) \quad (33)$$

then

$$dC^a/dt = g^{ab}(C^a, C^b)$$
$$dC^b/dt = g^{ba}(C^a, C^b) \qquad (34)$$

Thus it is seen that a reaction of two species has the effect of introducing a negative generation rate, or sink, that may simply be added to the generation term (species source), $g^k{}_n$, in the above equations. Generalization to reactions of more than two species is straightforward so that for the general case of reactive contaminants we may replace the simple source term, $g^k{}_n$, above by;

$$g^k{}_n + \sum_\alpha g^{k\alpha}{}_n + \sum_{\alpha,\beta} g^{k\alpha\beta}{}_n + \sum_{\alpha,\beta,\delta} g^{k\alpha\beta\delta}{}_n + \ldots \qquad (35)$$

where k,α,β,δ are contaminant species type indicies.

It must be remembered that all of these reaction-related terms depend upon the state of concentration in the zone n and thereby couple the contaminant dispersal equations nonlinearly.

The coefficient matrices of the thermal equations, (20a)(20b), are, in general, nonconstant (i.e., vary in time), nonlinear (i.e., depend upon zone temperatures, T_i, through both density and specific heat capacity), and implicitly coupled to the concentration equation through the dependency of both density and specific heat capacity on contaminant concentration.

The variation of density and specific heat capacity due to temperature and concentration changes is likely to be small, yet must be accounted for if bouyancy forces are important. It is reasonable to treat density and specific heat capacity constant in the thermal equations, (20a)(20b), yet account for density variations in the flow equations, (25)(26). This approximation is equivalent, in essence, to the Boussinesq approximation employed in the continuum formulation of bouyancy-driven equations and serves to reduce, but not eliminate, the nonlinearity of the system of equations and to uncouple the contaminant dispersal equation from the thermal and airflow equations.

Since equations (20a)(20b) and (26) are coupled nonlinear equations it may prove difficult to insure uniqueness of solution for bouyancy-driven flows analogus to Benard convection (the motion that results when a fluid is heated from below for Reynolds number above a critical value) and possibly other flows as well.

Equations (20a) and (20b) define the thermal behavior of an interzonal airflow network. They are identical in form to the general form of thermal element equations (that may be assembled to form systems of equations that govern the thermal behavior of complete thermal systems), and as such may be considered to be just another class of thermal element - an "airflow network element". This airflow network element may, then, be directly assembled, along with other building thermal elements (e.g. resistance elements, capacitance elements, conduction finite elements, MRT network elements, HVAC elements, etc.) to form a coupled system of equations that defines the coupled thermal behavior of the building system.

$$[C]\{dT/dt\} + [K]\{T\} = \{E\} \qquad (36)$$

where $\{T\}$ = vector of building system temperatures and includes zonal temperatures as well as other nodal temperatures in the complete building system model

$[C]$ = building system thermal capacity matrix

= $[M^z] + [c^e]$; the "direct assembly sum" of the zonal air capacitance matrix and all building thermal elements capacity matrices

$[K]$ = building system thermal conductance matrix

= $\{Cp^2\}[F^2] + [k^e]$; the "direct assembly sum" of zonal airflow conductance and all building thermal elements conductance matrices

$\{E\}$ = $\{E^2\} + \{q^e\} + \{q^{ext}\}$; the "direct assembly sum" of zonal direct gains, internally generated fluxes, and external fluxes due to convection and fluxes to the external boundaries of the building system.

The following procedures may be used to solve the collection of equations presented above,

Stepping through time;

Initialization

1. An initial building system temperature distribution is assumed;

   $\{T\}_o$ = assumed

Time Stepping Loop

2. The time step is incremented,

   $t_{n+1} = t_n + \delta t$

3. The first estimate of the temperature distribution at the next time step is made equal to the temperature distribution at the previous step;

   $\{T\}^i_{n+1} = \{T\}_n$

Airflow-Thermal Iteration Loop

4. The airflow matrix is evaluated, equation (25), (26), (27) and (28), using the current estimate temperatures, $\{T\}^i_{n+1}$.

   - airflow continuity may be checked, equation (29) and (30).
   - the airflow conductance $\{Cp\}[F^2]$ is assembled into equation (36).

5. The thermal equations (36) are solved (using an appropriate finite difference scheme) to obtain a better estimate of current temperatures, $\{T\}^{i+1}_{n+1}$ for the current boundary conditions, imposing current excitations (boundary conditions) and accounting for any changes in the system matrices [C] and [K].

6. If $\{T\}^{i+1}_{n+1}$ has converged to $\{T\}^{i}_{n+1}$, within acceptable tolerance, proceed to step 7, otherwise go back to step 4.

Contaminant Dispersal Solution

7. Solve the contaminant equation (29) (using an appropriate finite difference scheme).

8. Go back to step 2.

If airflow is a prescribed function of time (equation 25), then iteration will not be necessary.

If the airflow is dominated by forced convection, then convergence of the airflow-thermal iteration will be rapid, as forced convection has the effect of reducing the nonlinearity of thermal equations. Similarly, if heat transfer within the building system is dominated by other phenomena than airflow transfer then, again, convergence will be rapid. But as airflow becomes dominated by bouyancy-driven flow, and airflow heat transfer becomes a dominant mode of heat transfer, then convergence should be expected to be slower.

For multiple contaminants, including water vapor, step 7 above would simply be repeated for each contaminant. If the variation of water vapor, or any other contaminant, is great enough to cause significant changes in zone densities and specific heat capacities, the Boussinesq approximation may not provide adequate accuracy. These sources of nonlinearity could be accounted for within the interative loop above in step 5.

4.9 Multi-Node Models

The next extension of the one-node model is the two-node model. In this case, the space is divided into two zones, chosen to be representative of the important zone volumes, such as the occupied (lower) part of a space, or near known pollution sources, etc. The second zone (node) would be the balance of the space. The assumption is made that pollutant concentrations are uniform within each zone, but different from the other zone. Three such models will be discussed: 1) Two-chamber HVAC system model, 2) Sandberg's model [22], [23], [24] for ventilation efficiency, and 3) The m-p model of Ishizu [25]. Figure 8 shows a typical air distribution system.

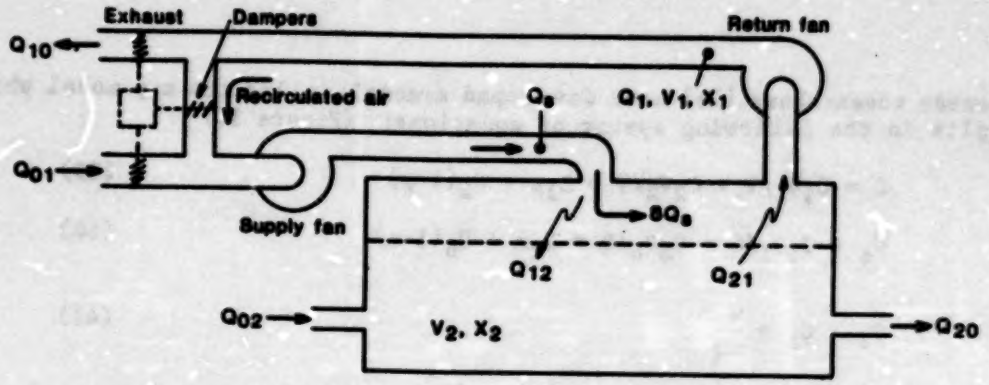


Figure 8. Typical Air Distribution System

A two-chamber model for the HVAC system results in equations which give ventilation efficiency, η_v:

$$Q_{10S} = S(1-R)Q_{01}\,[1 + RS + (RS)^2 + \ldots]$$

$$\frac{Q_{10S}}{Q_{01}} = \frac{S - SR}{1 - SR}$$

$$\eta_v = \frac{Q_{01} - Q_{10S}}{Q_{10}} = \frac{1 - S}{1 - SR} \qquad (37)$$

Q_{01} = flow rate of outdoor air

Q_{10S} = the amount of outdoor air that by-passes the occupied space and is exhausted

S = the fraction of the supply air which by-passes directly to the return inlet without mixing in the occupied zone

R = the fraction of the return air which is recirculated. The remainder (1-R) is exhausted.

Sandberg and Skaret [22-24] have developed equations for ventilation efficiency and a mixing factor. Sandberg's mixing factor, η, appears to be related to the stratification factor, β, by,

$$\beta = 1-S,\ \eta_v = \beta \qquad (38)$$

when R = 0

Figure 9 depicts examples of flows for various cases of idealized mixing.

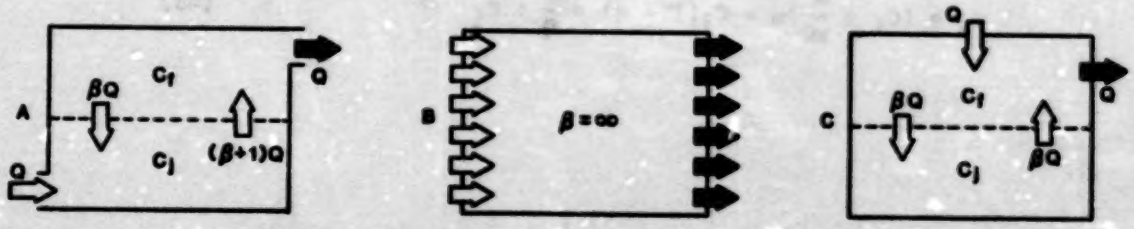


Figure 9. Ventilation Flow Configurations

Japanese researchers [25] have developed a model called the m-p model which results in the following system of equations: (Figure 10)

$$C = C_1V_1/V + C_2V_2/V = C_1p + C_2(1-p) \tag{39}$$

$$C_e = C_1Q_1/Q + C_bQ_b/Q = C_1m + C_b(1-m) \tag{40}$$

$$C_1 - C_i = \frac{G}{mQ} \tag{41}$$

where m = mixing factor
The mQ portion of the supply air mixes completely with the room air and the (1-m)Q portion by-passes without mixing [25].

p = position factor
Zone 1 is the region of volume pV where the pollutant diffuses completely. Zone 2 is the fresh air region of volume (1-p)V.

Q = volumetric flow rate of supply air

G = pollutant generation

V = volume of the room (V_1,V_2 represents volume of zone 1, zone 2)

C = average concentration for the whole room

C_e = concentration in the exhaust air

C_1,C_2 = concentration in the zone 1, zone 2

C_b = concentration in the by-pass air

C_i = concentration in the supply air

From equation (39) and (41), the concentration for the whole room is

$$C = (C_2 + \frac{G}{mQ})p + C_i(1 - p) = \frac{pG}{mQ} + C_i \tag{42}$$

and the exhaust concentration is

$$C_e = (C_i + \frac{G}{mQ})m + C_i(1 - m) = \frac{G}{Q} + C_i \tag{43}$$

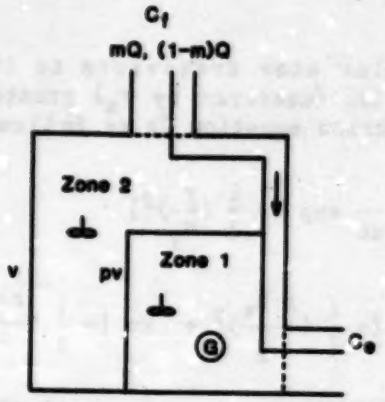


Figure 10. Basic Concept for Mixing-Position (m-p) Model

Since the average concentration is proportional to p/m, to make p small and/or to make m large can be a criterion for effective cleaning of the indoor air pollutants with a fixed number of air changes.

4.10 Transport Models

The models which describe how pollutants are transported into the environment from point sources have had attention in outdoor situations. This class of models could be used for predicting the local concentration of contaminants without having to solve the full equation (see section 5). The following discusses the possible use of these models in indoor conditions.

Atmospheric transport models are used to model the transport of pollutant emitted by stacks [26,27]. They predict downwind concentrations at any height, including ground level, for different atmospheric conditions and for various types of terrain. We will concentrate on those aspects of these models that may be applicable to indoor air quality modeling. The models, properly modified, will presumably be usable whenever indoor pollutants are emitted by identifiable point sources, for example, cigarettes, ovens, gas ranges, and open paint or solvent containers. Using these models for indoor conditions should be much less complex than for their original purpose because terrain need not be considered, air velocity and temperature gradients are very small if not negligible, photochemical reactions are unimportant and, unlike power plant plumes, indoor "plumes" would generally only rise by buoyancy and not as jets.

It will be necessary to model ceilings and walls, which obviously do not restrict outdoor plumes; however, ceilings play the same role as temperature inversion layers, which effectively limit the rise of plumes, and may be capable of being treated in a similar way. This is shown in figure 11, which depicts different plume types. Indoors one would expect either a horizontal spread from a pollutant source, if it is not a flame, or a nearly vertical rise until the plume reaches the ceiling, after which it would spread out as in the trapping or fumigating plume types (see figure 11) until it reaches the walls, where part would reflect back into the spreading plume while the other part descends. Absorption by surfaces would have to be taken into account.

The general plume diffusion model, illustrated in figures 12 and 13, assumes that after becoming horizontal, plumes obey Gaussian distributions

along the two perpendicular axes transverse to their flow, with the horizontal standard deviation (measured by σ_z) greater than the vertical (measured by σ_y). The diffusion equation is as follows [26]:

$$X(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z u} \exp\left[-\frac{1}{2}\left(\frac{Y}{\sigma_y}\right)^2\right] \cdot$$

$$\left\{\exp\left[-\frac{1}{2}\left(\frac{z-h_s}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+h_s}{\sigma_z}\right)^2\right]\right\} \qquad (44)$$

The variables are illustrated in figures 12 and 13. The model is valid for any consistent set of units. Wind speed must be replaced by an appropriate velocity for indoor use, for example, the rate at which the plume spreads horizontally at the ceiling.

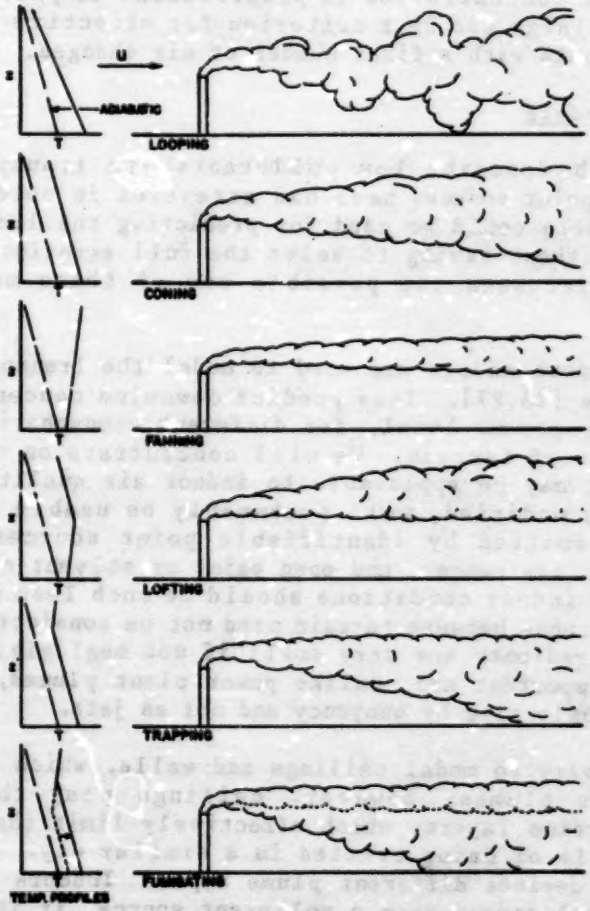


Figure 11. Plume types for various thermal stabilities. The top three with uniformly varying temperature with elevation: unstable, adiabatic (neutral), and stable. The bottom three are caused by discontinuities in stability of atmospheric layers. Note: T = temperature; z = height. (An adiabatic temperature gradient is one in which there is no net heat exchange between the plume and its surroundings).

The following equation is for plumes that do not rise:

$$X(x,y,z,h_s = 0) = \frac{Q}{\pi\sigma_y,\sigma_z u} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z}{\sigma_z}\right)^2\right] \qquad (45)$$

These equations can predict concentrations at various heights and distances from the sources, maximum concentrations, and where they occur. For example, the ground-level concentration calculated from equation 45) is:

$$X(x,y,0,h_s = 0) = \frac{Q}{\pi\sigma_x,\sigma_z u} \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \qquad (46)$$

The maximum concentration for a given x is found on the centerline.

$$X(x,0,0,h_s=0) = \frac{Q}{\pi\sigma_y,\sigma_z u} \qquad (47)$$

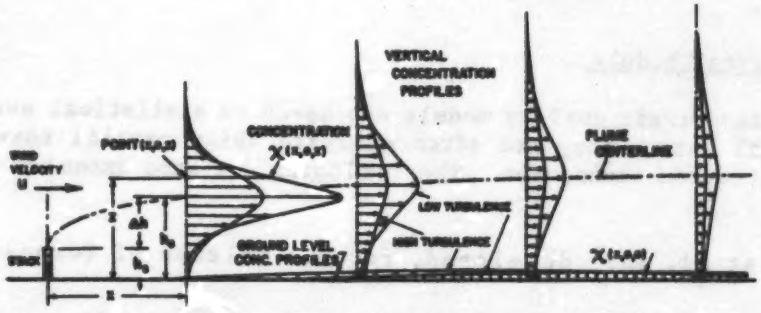


Figure 12. Plume concentration profiles and centerline location in the vertical xz plane.

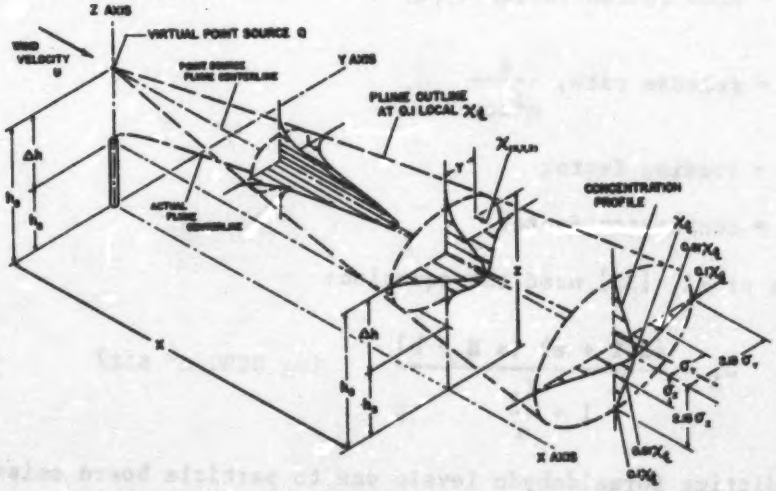


Figure 13. Three-dimensional concentration profiles of a nonrising point source and centerline of a rising plume for diffusion calculations at distance x.

As mentioned above, these equations would have to be modified for reflection and absorption by walls and ceilings.

There are specialized models to account for pollutants rising from multiple stacks [27]; these may be useful for multiple point sources of indoor pollutants.

Equations 44 and 45 may be modified for particulates by tilting the horizontal plume downward by an angle V_g/u, where the numerator is the terminal velocity of the particulate, and u is the wind speed. Terminal velocities are given in reference [26]. An effective plume height, h_{ep}, replaces h_e in the diffusion equation; it is given by:

$$h_{ep}(x) = h_e(x) - x \cdot V_g/u \qquad (48)$$

A different such equation must be used for each different value of V_g.

NBS has also done modeling of smoke movement in spaces, [28-31] which may also be usable for other pollutants. Smoke plumes in rooms from point source fires, and the plume's movement to other spaces have been considered.

4.11 Empirical Models

Empirical indoor air quality models are based on statistical evaluations of experimental data. They are often analyzed using partial correlation and linear regression techniques. The following are some examples of this type of model.

Pickrell et al. [32] developed, for the release of formaldehyde, the relation:

$$C = RLF \qquad (49)$$

where C = HCHO concentration (ppm)

R = release rate, $\frac{g}{m^2 day}$

L = loading factor

F = conversion factor

Anderson et al. [33] used the equation:

$$C_i = \frac{(d\,T + e)\,(a\,H + b)}{1 + \frac{I_c}{\alpha}} \quad (\text{mg HCHO/m}^3 \text{ air}) \qquad (50)$$

for predicting formaldehyde levels due to particle board emission.

where a,b,c,d,and e = empirical constants that are functions of the type and surface coating of the particle boards.

T = room air temperature (°C)

H = humidity (g H_2O/kg dry air)

I = air change rate (hr^{-1})

a = ratio of free particle board area in the room and total volume of the room (m^{-1})

In the range of 17-32°C (63-90°F), 5-13 g H_2O/kg air (.005-.013 lb H_2O/lb air) and 0.4-3 ACH, the model predicted the actual concentrations of formaldehyde well, with an average correlation coefficient of about 0.9 [33].

Gammage and Hawthorne [34] used the equation:

$$C = \frac{AS}{1.25\ V \cdot I} \qquad (51)$$

for relating the indoor concentration of formaldehyde to source strength and ventilation rate.

where: C = calculated HCHO concentration (ppm)

A = active wall area emitting formaldehyde (m^2)

S = emission rate ($\frac{mg}{m^2\ hr}$)

I = rate of air exchange (h^{-1})

V = room volume (m^3)

1.25 = conversion factor

Dockery and Spengler Model [35]

For respirable particles and sulfates, Dockery and Spengler developed empirically the following expression for the exposure to particulates:

$$E = t_{home}\ C_i + t_{out}\ C_o + t_{other}\ (C_i + N_{smoke} \times 20) \qquad (52)$$

For sulfates, the average exposure, e, is given by

$$e = \frac{t_{in}\ C_i + t_{out}\ C_0}{t_{tot}} \qquad (53)$$

In equation (52) and (53),

t_{home} = time spent in home

t_{out} = time outdoors

t_{in} = time spent indoors

t_{other} = time spent indoors away from home

t_{tot} = total sample length

N_{smoke} = number of smokers to which a participant was exposed

and C_i and C_o are the average concentrations in the respective areas.

In later work [36] Dockery and Spengler developed the following series of equations:

$$\bar{C}_i = P\bar{C}_o + \frac{S}{q} \qquad (54)$$

for the average indoor concentration, where the overbar indicates 24-hour average values.

In equation (54)

C_i = concentration

$P = B_1 + B_2 (A)$

A is an indicator variable for fully air conditioned
B's are empirically determined

$$\frac{S}{q} = B_3 (N_{cig}) + B_4 (AN_{cig}) + B_s (A) + B_o$$

where N_{cig} = estimated number of cigarettes smoked indoor per day.

For sulfates, they used:

$$\frac{S}{q} = B_3 (N_{cig}) + B_4 (AN_{cig}) + B_5 (G) + B_6 (AG) + B_7 (A) + B_o \qquad (55)$$

where G is an indicator variable for cooking fuel
(1 for gas, 0 otherwise) and

B coefficients are determined by regression on indoor-outdoor concentration data on the measured parameters.

5. Convection Simulation Models

Indoor air contaminant migration from sources to various zones and/or from zone to zone in the building by assuming that the contaminant concentration is constant throughout each zone, or there is perfect mixing in the zone, has been covered above. While this assumption may be considered valid for each zone where air is well recirculated and strong localized sources and/or sinks of the contamintants do not exist, observed data often reveal

significant stratification and localised concentration gradients, even in a well ventilated rooms.

Since the major portion of the mixing is accomplished by the convection process, the molecular diffusion part being extremely small (approximately the order of 0.1 air changes per hour), the imperfect mixing problem requires that one solve for the convective transfer of contaminants in the room as affected by the forced ventilation and natural circulation due to thermal draft.

The equation of air motion that governs the conventional room convection process is

$$\rho\frac{\partial\vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} = -\nabla p + \vec{\tau} + \vec{F} \qquad (56)$$

where ρ = density

$\vec{u}$ = velocity vector

p = pressure

t = time

∇ = mathematical symbol for gradient

The terms of this equation of motion expressed per unit volume of fluid element are, from left to right:

Rate of momentum increase,
Rate of momentum gain by convection,
Pressure force on element,
Rate of momentum gain by viscous transfer, and
Body force

Introducing an operator to include the effect of convection D/Dt such that

$$D/Dt = \frac{\partial}{\partial t} + (\vec{u}\cdot\nabla) \qquad (57)$$

the above equation of motion takes a form of the familiar Newton's equation

$$\rho\frac{D\vec{u}}{Dt} = -\nabla p + \vec{\tau} + \vec{F} \qquad (58)$$

Moreover, the viscous transfer term may be expressed by using the dynamic viscosity such that

$$\vec{\tau} = \mu\nabla^2\vec{u} \qquad (59)$$

Another important relationship between the hydrostatic pressure gradient and air density and that between the air density and air temperature lead to the form commonly used for the buoyance force

$$\vec{F} = g\beta T\vec{i}_g \qquad (60)$$

where g = gravitational acceleration

T = temperature above an arbitrary datum point

β = the coefficient of thermal expansion

and $\vec{i}_g$ = the unit vector in the direction of gravity.

Thus the momentum equation for the convection cannot be solved without the space distribution of air temperature, which in turn requires a solution for the energy balance equation (neglecting the nonlinear viscous heating terms), such as

$$\rho c \frac{DT}{Dt} = k\nabla^2 T + q_h \qquad (61)$$

where c = specific heat of air

k = thermal conductivity of air

ρ = air density

q_h = volume heat source strength

After equations (58) and (60) are solved simultaneously, they provide the space distribution of u, which is essential for the contaminant mass balance equation

$$\frac{DC}{Dt} = \nabla\cdot(D_v \nabla C) + q_c \qquad (62)$$

where D_v = diffusion coefficient of the contaminant in the air and q_c is the volumetric contaminant source strength.

Note that the forms of equations (61) and (62) become identical if the thermal diffusivity $k/\rho c$ and the mass diffusion coefficient D_v are constant. In addition there exists an additional and important equation expressing the continuity of air mass such that

$$\nabla\cdot\vec{u} = 0 \qquad (63)$$

In order to predict the contaminant concentration C in the space, it is essential that the space air velocity vector u and space air temperature T be solved simultaneously by equations (58), (61) and (63). The solution must also satisfy prescribed initial and boundary conditions and overall mass balance relationships.

While the initial conditions for $\vec{u}$ may be set equal to zero and T and C may be set at the mean room values, the boundary conditions are specific to room configuration, air supply and return systems, and heat transfer characteristics of the room envelope surfaces. The velocities are usually

considered zero except where air intakes and outlets are located. Temperature and concentration at the supply air inlet must also be provided, whereas those at the outlet are to be calculated to satisfy the overall energy and mass balance such that total energy and mass generated in the room is equal to those ventilated out by the exhaust air.

The temperature boundary conditions are usually more complicated, requiring detailed surface heat balance calculations involving

- o heat conducted into the solid surfaces
- o long wavelength radiative heat exchange with the surrounding surfaces
- o short wavelength radiative heat input from the sources such as solar heat gain and/or lighting systems
- oheat generated at surfaces, such as heat sources, human bodies, appliances, lighting fixtures, etc.
- o heat convected into the air
- o heat stored in the air
- o heat stored by solids

Boundary conditions on the contaminant concentration must also include the emission, adsorption and desorption characteristics of the boundary surface.

Although equations (57) through (62) provide the fundamental relationships to determine convective mixing of the indoor air pollutants, actual solution of these equations applicable to realistic building situations are not easy because the room air motion is highly turbulent and three dimensional. Its boundary surfaces are complicated by the irregular geometries of room architecture and internal furnishings. Very difficult and time consuming numerical calculations using finite difference and/or finite element methods are necessary to solve these equations together with additional equations for such properties as turbulent kinetic energy and turbulent energy dissipation rate, details of which are not warranted in this report. Numerous publications relating to the solution of room convection problems are available, a comprehensive summary of which has been published by Kaizuka [37].

Only recently a comprehensive treatise of turbulent room convection and its effects upon the contaminant mixing and ventilation effectiveness have been given by Ishizu [38,39], but only for a simple rectangular room with a simple ventilation system. A similar solution for a completely sealed chamber has also been given by Rehm and Baum for the simulation of aerosol migration at the onset of a room fire [40,41]. Some of Ishizu's calculation results, transcribed from his published work on two dimensional solutions as well as his unpublished work on three dimensional analysis, presented at a recent NBS meeting, are illustrated in the attached figures.

Ishizu analyzed a cubic room as shown in figure 14, when the ventilation inlets, outlets and contaminant point source are moved around to see the effect of air mixing and ventilation effectiveness.

Figures 15 and 16 depict the air flow velocity vectors and iso-concentration contours in the mid-section (cross section ABC of figure 15) of the room for case 1 when the air is supplied at the upper left corner of

analysis, the contaminant source is located above the middle of the floor, indicating a relatively stagnant condition in the middle and upper right corner of the room. Figures 17 and 18 show the similar plots for case 2 when the air inlet was moved to the center of the ceiling, whereas figures 19 and 20 show case 3 when the air inlet was moved near to the exhaust side of the room indicating that a large portion of the room is unvented. Figures 21 and 22 represent iso-concentration contours for cases 4 and 5 when the sources are moved to the left corner and to the front of the air outlet. Using the results of these calculations Ishizu determined the mixing factor and ventilation effectiveness by integrating the local concentration data as follows:

$$m = \frac{Qt}{V} \Big/ \ln \frac{(C_o - C_i)}{(C - C_i)} \tag{64}$$

$$E_v = \frac{G}{(\bar{C}_\infty - C_i)Q} \tag{65}$$

where m = mixing factor

E_v = ventilation effectiveness (the reciprocal of Ishizu's $\frac{P}{m}$) see eq. (23)

G = pollutant generation rate

Q = ventilation rate

V = room volume

t = time

C_o = initial pollutant concentration at t = 0

C_i = pollutant concentration of supply air

$\bar{C}_\infty$ = room average pollutant concentration at time t

C = steady state room average pollutant concentration

Figure 23 summarizes the results of Ishizu's analysis where cases 6 through 10 are also presented to compare the similar analysis previously reported [25] for the two dimensional room calculations.

This figure reveals the following interesting observations:

1. Mixing factor is independent of the location of the pollutant sources and only the function of the location of the ventilation system.

2. Three dimensional calculations result in considerably different results from the two dimensional solution, although the general trend of ventilation efficiency is the same, being highest when the source is near the exit and lowest when the mixing factor is the smallest.

3. Although generally the mixing factor is larger as the airflow path in the room is longer, case 2 mixing is slightly higher than case 1 indicating the complex nature of three dimensional air flow.

One of the intriguing results of the Ishizu analysis is shown in figures 24, 25 and 26, which are the logarithmic plots of local pollutant concentration decay with respect to time determined at selected points for cases 1, 2 and 3 when the pollutant emission was suddenly stopped at the source. Also indicated in those figures are the logarithmic slope of the room concentration decay representing perfect mixing, (n = 1). Although the logarithmic concentration decays show almost identical slopes for all the points investigated for a given room, they differ from case to case, case 2 being the closest to the perfect mixing. That the local concentration decay trends are identical, independent of their location in the room, is somewhat difficult to believe, since some of the points in the ventilating air stream should experience higher rates of decay than those in the stagnant area.

Although all of these calculations were performed for isothermal room conditions, without regard to thermal convection, figures 27 through 32 depict results of calculations where the energy equation was simultaneously solved to include the thermal convection effect. Temperature and concentration profiles at cross section ABC of the room (figure 14) are shown in figures 27 and 28 respectively in the case when the cold air supplied to the room with the floor having a warmer temperature than the average. Figures 29 and 30 represent the similar plots when the hot air was supplied to the room having the normal ambient temperature. Significant changes in the concentration contour lines are evident. Also interesting are plots of local concentration decay at several selected points in the room as shown in figures 31 and 32. The mixing factors are considerably lower when the cold air is supplied from the ceiling rather than the warm air, which is contrary to the conventional understanding of the problem.

Although very interesting and comprehensive, the Ishizu calculations have several problem areas which need attention before the results can be fully accepted and extrapolated for general use:

1. The overall grid size used for the calculations was 10x10x10, in which each boundary takes up two grids, is far too coarse to obtain an accurate assessment of realistic room air convection and pollutant distribution. This may be the reason for the peculiar results, such as shown in figures 24, 25 and 26.

2. Inlets and outlets are two grid sizes and too large and unrealistic in reference to actual room situations.

3. The inlet air velocity profile was assumed straight downward, which is not common in actual air diffuser systems.

4. Boundary layer calculations were oversimplified, assuming zero gradients for velocity as well as for the temperature.

5. Mixing factors and ventilation effectiveness are not yet available for the non-isothermal situations.

6. The validation of calculated concentration contours with the measured data was done only for a 40 cm cube model and the agreements between the calculated and observed velocity data are only quantitative (figure 33).

7. The model is restricted to extremely simple and elementary geometry and internal furnishings are not included.

8. Only a single point source is treated.

9. The current model can not handle natural ventilation when the supply air inlet velocity is zero.

10. Presently the momentum equation is coupled only to the energy equation, ignoring the fact that the mass is, in reality, also coupled because the pollutant concentration gradient also causes the buoyant force, such as in the case when a heavy pollutant gas settles to the lower portion of the room.

In order for the convection model to be able to provide accurate prediction of the local concentration of a pollutant, the following research must be carried out:

1. Ishizu's calculations must be validated with much finer grid. This entails the vectorization of the calculation algorithms to expedite the computational speed on very efficient modern computers such as CRAY or CYBER (see for example [40,41]).

2. Improvement of algorithms is needed to handle more realistic boundary conditions, especially those representing air inlets and outlets.

3. Employment of finite element type calculations is needed, rather than the finite difference approach, so that complex room geometries, especially those pertaining to the internal obstructions, can be handled.

4. Through rigorous experimental investigations, reliable data for checking the accuracy of the calculated concentration distribution, turbulent energy and turbulent energy dissipation rate must be obtained for typical rooms with more representative air inlets and outlets.

5. The two-equation model used by Ishizu should be extensively compared to other simpler models to see under what conditions the latter may be adequate.

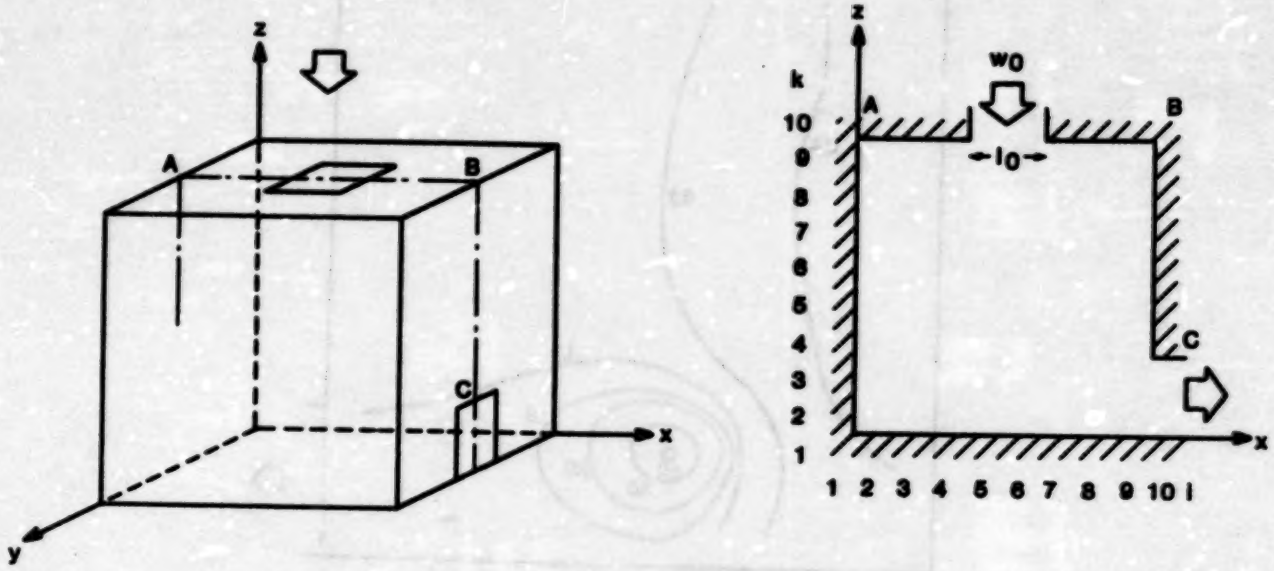


Figure 14. The room configuration, cross section ABC and grid design used by Ishizu

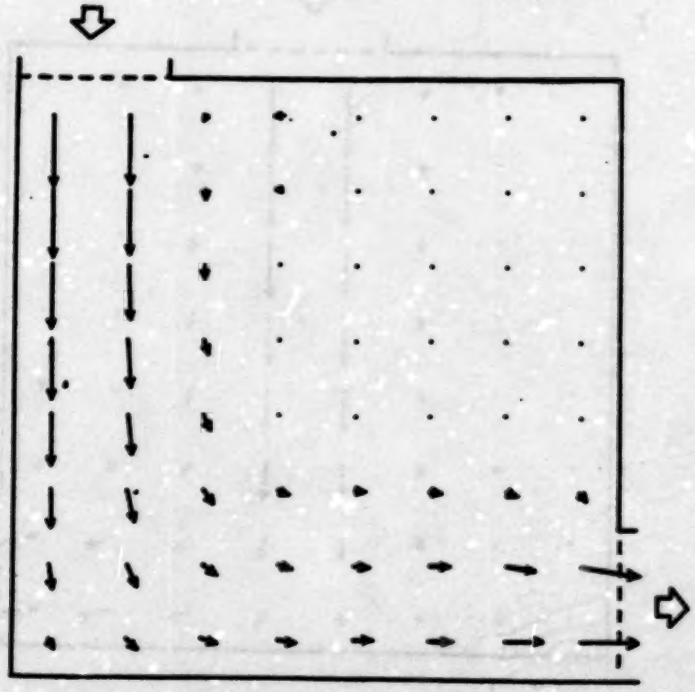


Figure 15. Velocity vectors on cross section ABC when the air inlet is at the leftmost position in the ceiling (case 1)

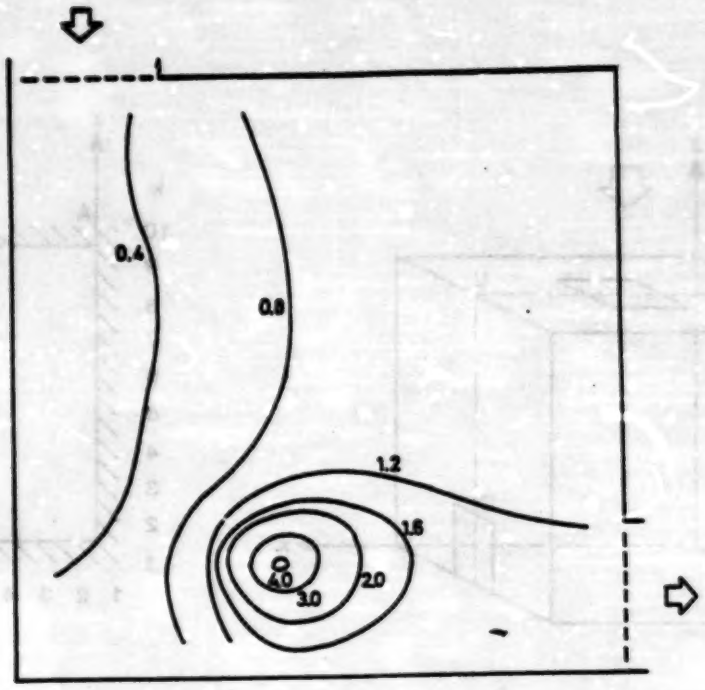


Figure 16. Pollutant iso-concentration contours in cross section ABC for case 1

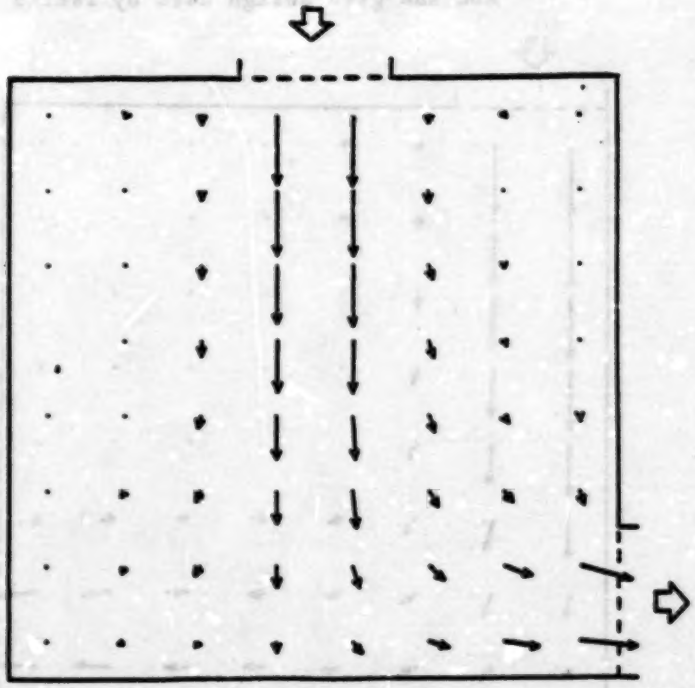


Figure 17. Velocity vectors on cross section ABC when the air inlet is at the center of the ceiling (case 2)

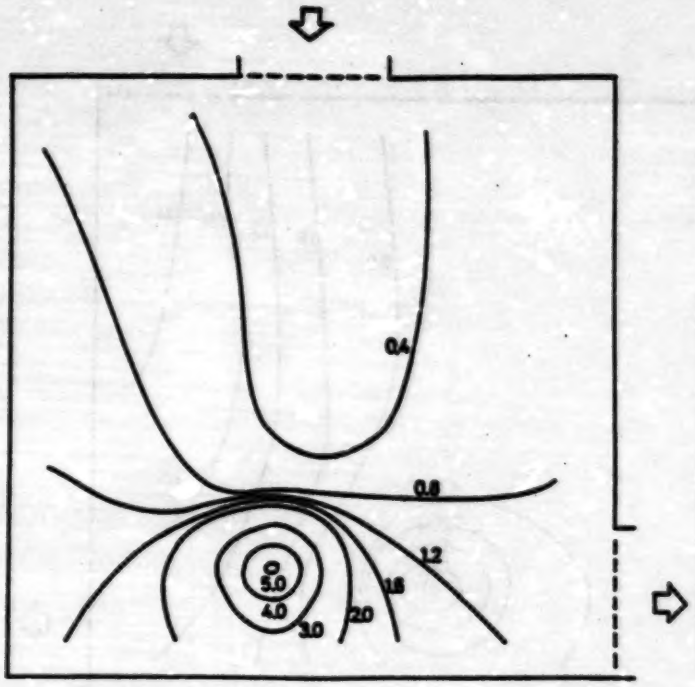
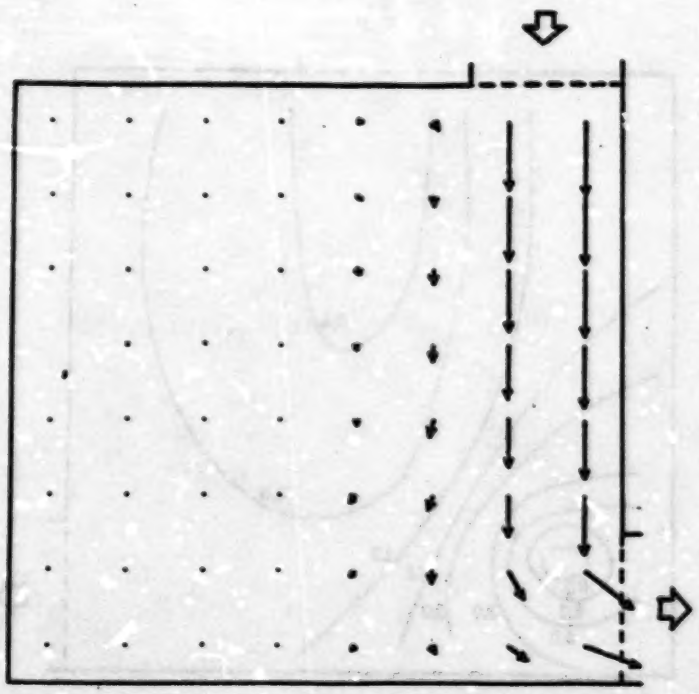


Figure 18. Pollutant iso-concentration contours in cross section ABC for case 2



Figures 19. Velocity vectors on cross section ABC when the air inlet is at the rightmost position in the ceiling (case 3)

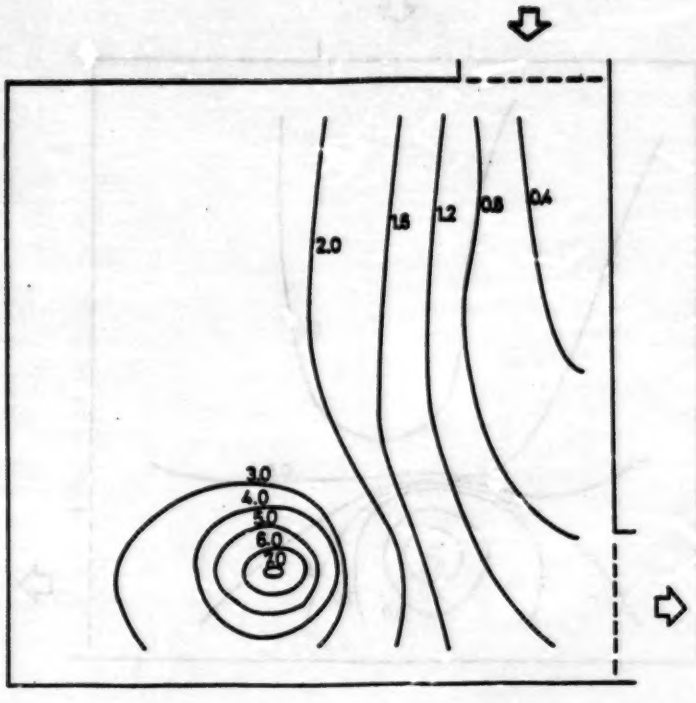


Figure 20. Pollutant iso-concentration contours in cross section ABC for case 3

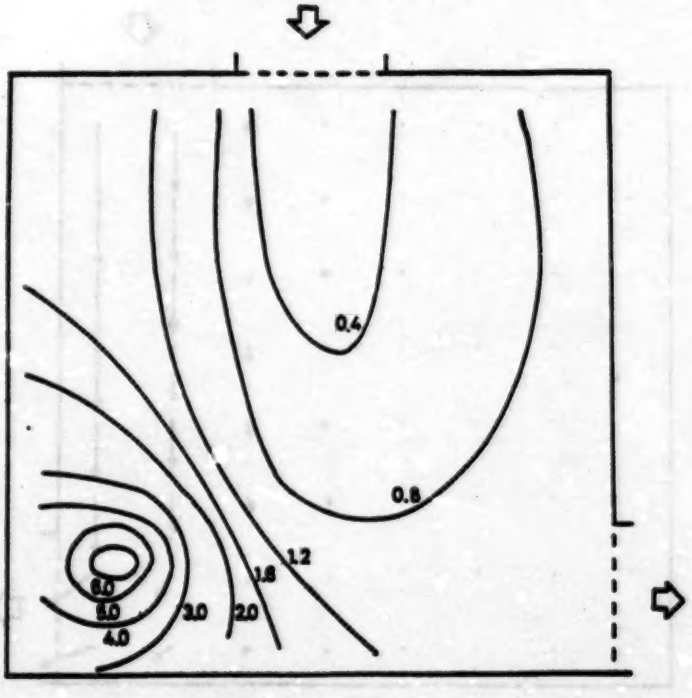


Figure 21. Pollutant iso-concentration contours in cross section ABC for case 2 except that the source is moved to the lower left corner of the room (case 4)

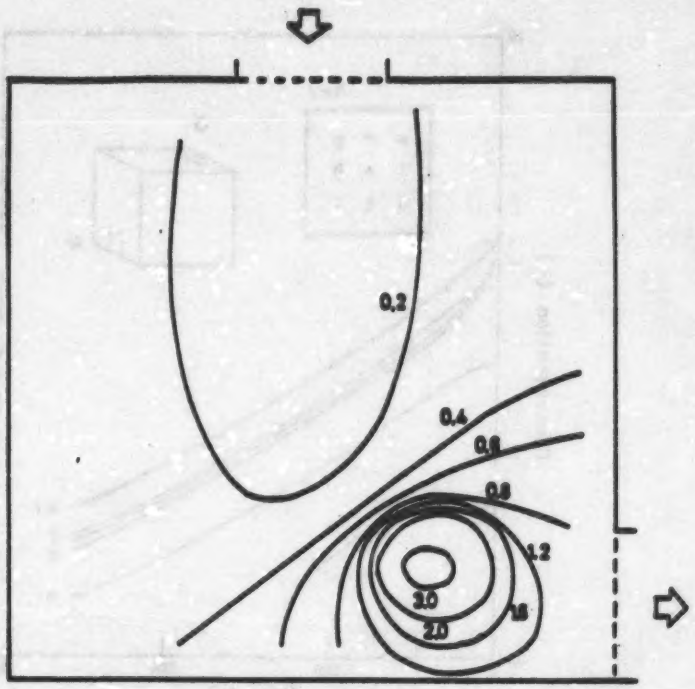


Figure 22. Pollutant iso-concentration contours in cross section ABC for case 2 except that the source is moved to the lower right corner near the air outlet (case 5)

Case	1	2	3	4	5	6	7	8	9	10
m	0.72	0.75	0.42	0.75	0.75	0.42	0.22	0.11	0.22	0.22
E	1.47	1.12	0.53	0.78	2.70	3.45	0.32	0.10	0.20	7.14

Figure 23. Mixing factors and ventilation effectiveness for three dimensional calculations (cases 1 through 5) and two dimensional analysis (cases 6 through 10)

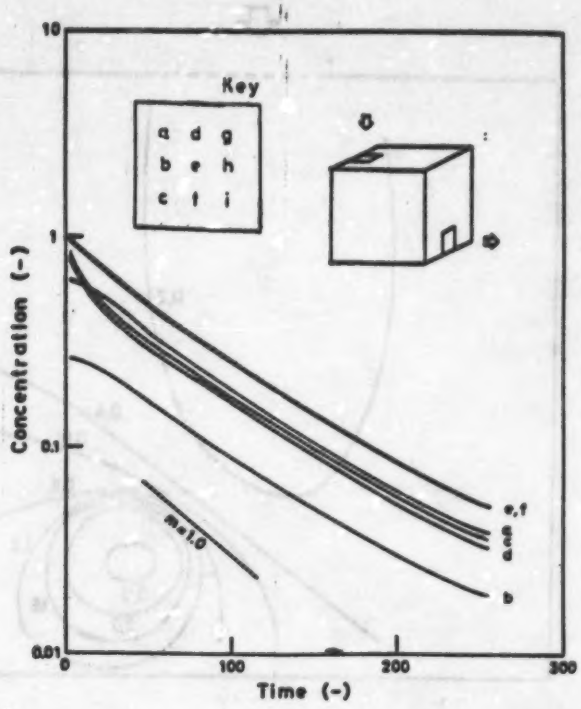


Figure 24. Logarithmic pollutant concentration decay at various positions in the room under case 1 ventilation conditions

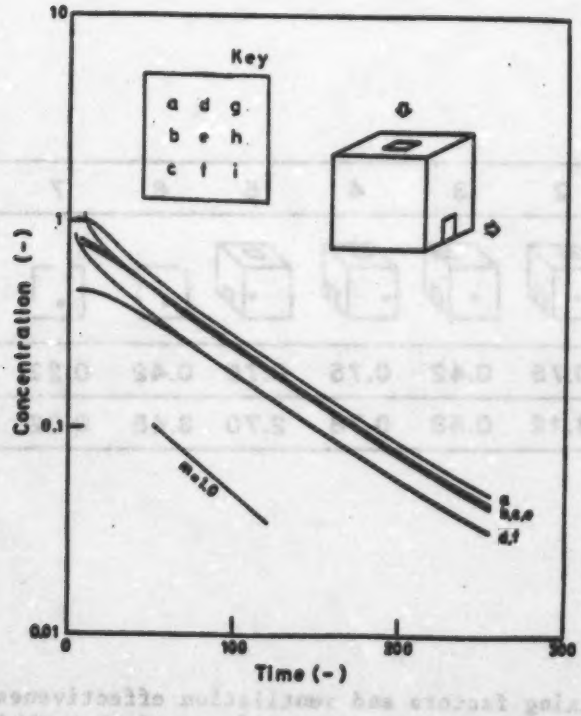


Figure 25. Logarithmic pollutant concentration decay at various positions in the room under case 2 ventilation conditions

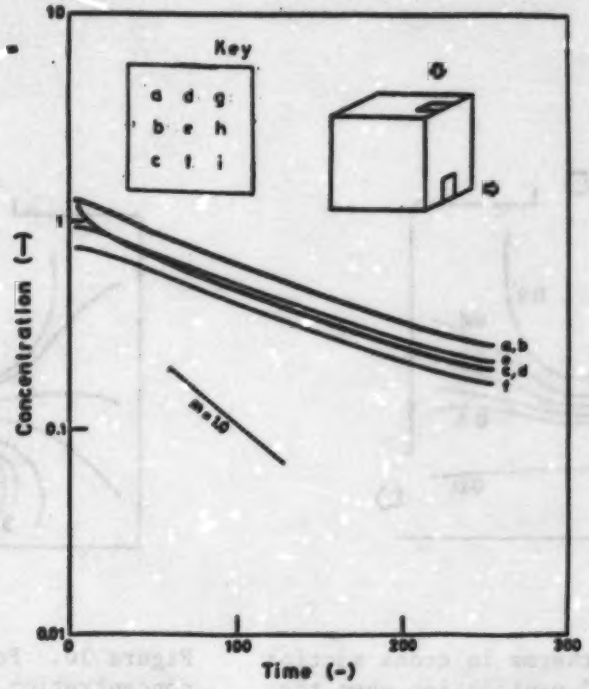


Figure 26. Logarithmic pollutant concentration decay at various positions in the room under case 3 ventilation conditions

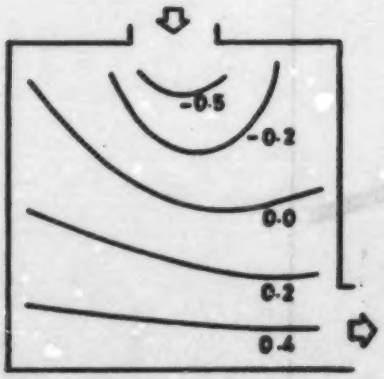


Figure 27. Isotherms in cross section ABC under case 2 ventilation when the supply air temperature is colder than the floor.

Figure 28. Iso-concentration contours in cross section ABC under case 2 ventilation when the supply air temperature is colder than floor.

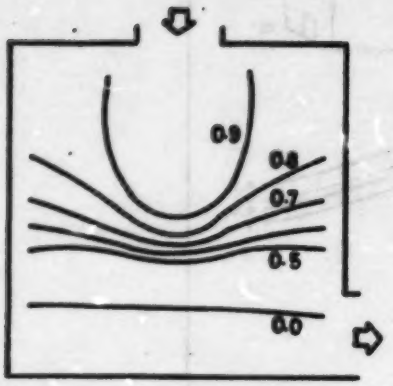


Figure 29. Isotherms in cross section ABC under case 2 ventilation when the supply air is warmer than the floor.

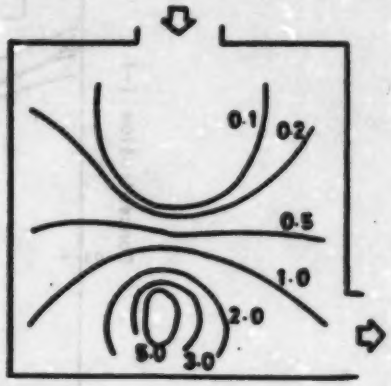


Figure 30. Pollutant iso-concentration contours under case 2 ventilation conditions when the supply air is warmer than the floor.

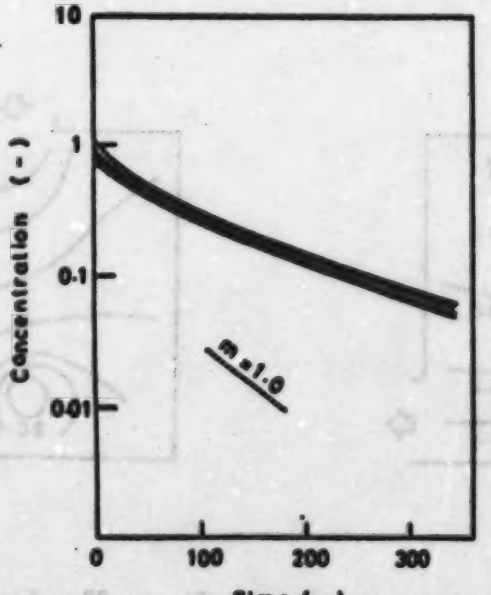


Figure 31. Logarithmic concentration decay at selected locations in the room ventilated with cold air.

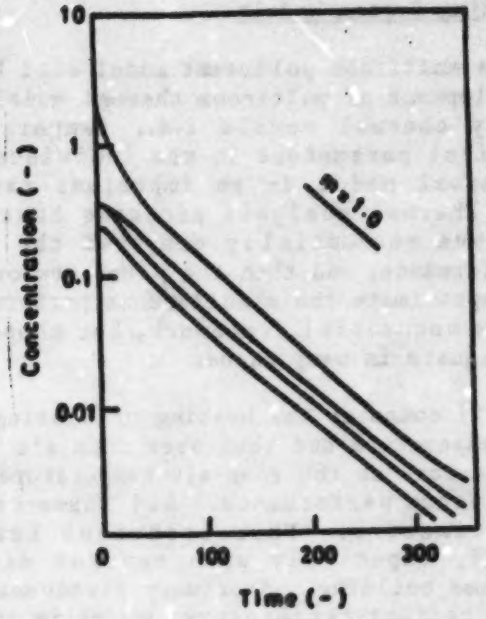


Figure 32. Logarithmic concentration decay at selected locations in the room ventilated with warm air.

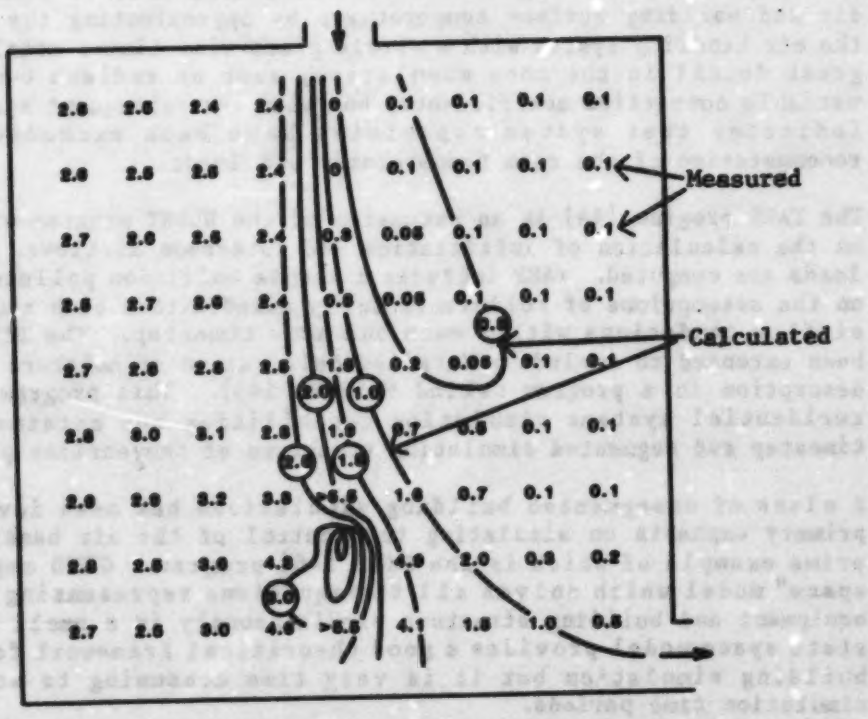


Figure 33. Comparison between the measured and calculated velocities and concentrations in cross section ABC under case 2 conditions.

6. Multi-room Building System Models

The development of a multiroom pollutant model will be based on procedures learned in the development of multiroom thermal models. In many cases the values computed by thermal models i.e., temperature, humidity, and airflows, are critical parameters in the individual pollutant models. Therefore the thermal model is an important part of the multiroom pollutant model. Thermal analysis programs have traditionally been segmented. They have sequentially computed the room loads, the air handling system performance, and then the plant performance. Various means have been used to approximate the simultaneous performance of room, system, and plant within the sequential framework, but these approximations are believed to be inadequate in many cases.

The DOE-2 program [42] computes the heating or cooling loads of rooms at a constant room air temperature and then uses room air temperature weighting factors to adjust the load as the room air temperatures change according to the simulation of system performance. All these calculations are made using a one hour timestep. This technique has the advantage of computational speed, especially when several different systems are simulated for the same building. A primary disadvantage is the inability to compute the mean radiant temperature, which is important for comfort analysis.

The BLAST program [43] uses the heat balance method where the room loads are computed by solving the simultaneous heat balance equations for room air and building surface temperatures by approximating the performance of the air handling system with a simple piece-wise linear model. This allows great detail in the room simulation, such as radiant temperatures and variable convection coefficients, but when the subsequent system simulation indicates that system capacities have been exceeded there is no recomputation of the room temperatures and loads.

The TARP program [44] is an extension of the BLAST program with an emphasis on the calculation of infiltration and interroom airflows. Only the room loads are computed. TARP includes a simple multiroom pollutant model based on the assumptions of pollutants fully mixed within each room and constant airflow conditions within each one hour timestep. The TARP program has been extended to include a detailed calculation of moisture absorption and desorption in a program called MADTARP [45]. This program includes some residential systems simulation capabilities but retains the one hour timestep and segmented simulation structure of the earlier programs.

A class of unsegmented building simulations has been developed with a primary emphasis on simulating the control of the air handling system, a prime example of which is the GEMS [46] program. GEMS employs a "state space" model which solves all the equations representing the controls, equipment and building structure simultaneously in a small timestep. The state space model provides a good theoretical framework for solving the building simulation but it is very time consuming to solve for long simulation time periods.

The HVACSIM+ program [47] reduces computation time by using different timesteps for different components being simulated. This program emphasizes the modular nature of building/HVAC components and employs a

complex system of modular equation solving. Computer execution times are still much longer than for the simpler segmented programs.

7. Future Pollutant Algorithm Development

As seen above, not all pollutants are well enough characterized to adequately model source strengths or interactions with other materials in space. A general summary of needed research is given for those pollutants which are considered in the scope of this project. Further refinement and definition of these factors would facilitate greater utility of the prediction models to be developed in this project.

Radon - The source strength models are needed. Currently there is no known method of assessing a situation (a residence, for example) knowing its location and construction details, etc. and being able to predict radon source strengths. Much is known about the geography of "hot spots" and methods of radon entry, but more work is necessary. Good models exist on daughter production from radon in spaces. Work has also been done on the interaction of daughters with particles in air and measuring attached and unattached fractions of daughters. However, more work is needed on this interaction with particles, space charging, and the effects of high performance air cleaners. These results are needed in particular for predictions of health effects resulting from the application of various control options.

Formaldehyde - HCHO has been the focus of considerable work on emanation rate modeling. Further work would be helpful on the effects of various barriers (paints and films) on the emanation rates. Also the effects of room air humidity interactions are not well enough known, as well as the effects of absorption and desorption in and from building materials and furnishings.

Nitrogen oxides - As seen above, NO_2 has been extensively studied in a number of specific cases (ranges, with various cooking loads, space heaters, tuned in particular ways, etc.). However, it is not yet possible to predict the NO_2 generated from a variety of cases without measuring each. Prediction models are needed. In addition, laboratory and field tests have indicated that NO_2 reacts with the environment in the unpredictable way. This also needs better predictive models.

Tobacco smoke particles - If it is decided that $\pm$ 20% is not accurate enough for a cigarette emission rate of particulate matter, further quantification of this rate is needed. Since the rate varies with different brands and smoking habits, it is felt that averages will have to be used in the models, so no further work is recommended now. On the other hand, the particle size and composition of the particles probably have significant effects on health. Therefore better quantification of those factors is indicated. In addition, more information on particulate behavior in electric fields is needed. The effects of aging of smoke with time may also need refinement in the future.

Carbon Dioxide - CO_2 sources and movement within spaces seems to be complete enough for modeling.

Carbon Monoxide - CO needs better methods of predicting its source strengths from gas ranges and combustion heaters under the wide variety of combustion situations.

Water Vapor - The source strength of water vapor seems well enough known but its absorption and desorption into and from building furnishings and construction materials needs better quantification, as well as its effects on various pollutants.

8. Future Model Development

Subsequent work will involve expanding the existing framework based on the extensive NBS Thermal Analysis Research Project (TARP) which includes a general pollutant model. The expansion will be confined in phase 2 to residential situations. Specific known pollutant algorithms will be introduced, involving complex sources and emanation rates. Further development of the environmental and operational algorithms will be undertaken. It is planned to include several pollutants in the inputs for residences with central forced air HVAC systems. The outputs will be confined to well mixed situations and single node, multiroom cases. Research will be initiated on a 2 node model and its integration into the extensive existing thermal models, so these interactions can be added, when work is complete, at a later stage.

Work will be initiated on the convection model for a single space, predicting concentrations as a function of time in a three dimensional grid of the space. Single point sources of contaminants will be covered, as well as multiple point sources. Single and multiple area sources will also be studied. It is not envisioned at present that a general convection model can be incorporated in a comprehensive indoor air quality model. However, studying the predictions of general convection models can give indications of the limitations of simpler indoor air quality models and potentially lead to simpler multi-node models which can take into consideration poor mixing and ventilation effectiveness. It may also be possible to use room convection models in conjunction with multi-zone simulation models. In this case, the multi-zone simulation models would generate the boundary conditions to be used in the convection models.

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